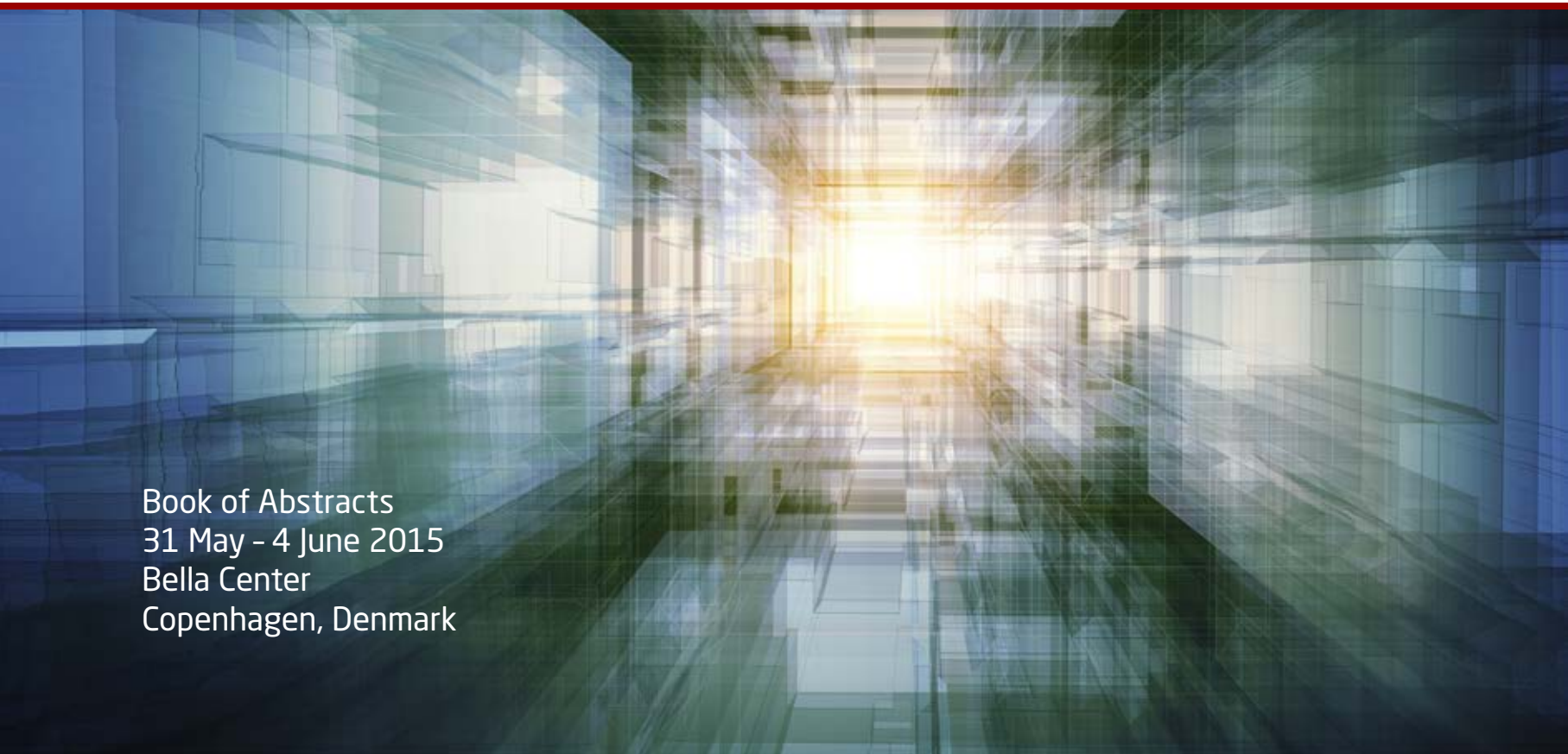
PSE2015 ESCAPE25

12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering



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Preface

It is our great pleasure to present the Book of Abstracts for the joint event of the 12th International Symposium on Process Systems Engineering (PSE) and the 25th European Symposium on Computer Aided Process Engineering (ESCAPE) in Copenhagen, Denmark. This conference features a variety of contributions from academia and industry highlighting the core products of the PSE/CAPE community. These contributions highlight the influence of process systems engineering to sustainability and define the future challenges for the community.

This conference marks the 25th anniversary of the ESCAPE-series and the 12th PSE conference. The PSE series is a triennial conference, which has been held since 1982, organized on behalf of the international PSE Executive Committee with representations from countries from the Asia Pacific, Europe and the Americas. The annual ESCAPE series started in Elsinore, Denmark in 1992 and is organized on behalf of the CAPE working party of the European Federation of Chemical Engineering. Both symposia serve as a forum for engineers, scientists, researchers, managers and students from academia and industry to show the progress being made. They also provide platforms for the discussion of the challenges being faced and the developments being made in the application of methods, algorithms and tools to solve this wide range of problems.

The PSE-2015/ESCAPE-25 joint event includes a large number of keynote lecturers from industry and academia as well as four plenary lectures covering topics on globalization, energy, environment and health from well-known experts from all over the world. Presentations will cover a wide range of topics: modelling, numerical analysis and simulation; mathematical programming (optimization); cyber-infrastructure, informatics and intelligent systems; process and product synthesis/design; process dynamics, control and monitoring; abnormal events management and process safety; plant operations, integration, planning/scheduling and supply chain; and finally, enterprise-wide management and technology-driven policy making. These presentations will also include the following domain applications: molecular, biological, pharmaceutical, food, energy, and environmental systems engineering.

This book contains abstracts of 544 contributions distributed in plenary and keynote lectures, oral presentations, and poster presentations. These numerous contributions are organized first by tracks and then by identification number (given in square brackets). To ensure easy navigation, there are two indices included at the end of the book: an index of authors and an index of abstract numbers. The index of authors lists all authors according to last name and the abstracts that they are associated with. Also, corresponding author emails are given in brackets for the corresponding author of each abstract (these are indicated in the abstracts with an asterisk). The index of abstracts simply lists the abstract number, in ascending order, and the page it can be found on. All presentations that will occur at the conference can thus be found by author, track or submission number.

We would like to thank all the authors for their work and timely submission. Some of the abstracts have been modified to fit the format of the book of abstracts. We hope the contents of this book serve as a valuable reference during the conference and as a record of the joint PSE-2015/ESCAPE-25 conference.

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Editors of the Book of Abstracts

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Plenary

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Multi-Level Design of Process Systems for Efficient Chemicals Production and Energy Conversion

Kai Sundmacher

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In the past decades significant progress in increasing the productivity, selectivity and sustainability of chemical production and energy conversion processes has been made. Nevertheless, in order to cope with the challenges of the future, breakthroughs in process systems engineering are necessary in order to find “dream processes” for synthesizing chemicals and transforming energy, to enable the transition from fossil fuels and petrochemical feed stocks to renewable materials and energy, to close carbon dioxide cycles, to enhance efficiency significantly, and to incorporate new functionality in materials and products.

For this purpose, new scientifically founded systems engineering approaches need to be developed, able to deal with the inherent multi-level structure of any production system. Very efficient process systems might be designable if engineers succeed to consider all essential levels involved in the process system hierarchy, namely the molecular level, phase level, process unit level and plant level [1]. But any multi-level design strategy will be successful only if mathematical process models, computer experiments and wet-lab experimental data are closely combined. Thereby, advanced quantitative understanding of complex process systems can be attained which will open new paths for translating scientific results into practical solutions.

In the present contribution, a model-based methodology is presented which derives process design decisions at different levels of the process hierarchy under consideration of various process inten-sifi--ca-tion options. This approach integrates optimal experimental design, process synthesis and process analysis. The proposed methodology is demonstrated for selected challenging process design tasks, e.g. Diels-Alder synthesis in organic solvents [2], alkene hydroformylation using homogeneous Rhodium catalysts [3], shape-selective crystallization of particles [4], and on-board hydrogen production for fuel cell vehicles [5].

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A Multidisciplinary Hierarchical Framework for the Design of Consumer Centered Chemical Products

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New consumer products such as personalcare products, mobile phones, tablet computers, smart windows, LED lamps, EV batteries,thin film solar cells, printed RFID and medical devices, are being introducedto the market at an increasingly rapid pace. This is driven partly by consumerdemands and partly by the emergence of new molecules, nanomaterials, advancedmaterials, and innovative processing technologies. Another contributing factoris the promotion of entrepreneurship by governments and academic institutions inboth developed and developing countries. This presentation describes aframework for the design of chemical products. It is consumer centered ensuringthat the consumers' wants and needs are met. It is hierarchical covering the designactivities level by level with additional details and finer scales whilekeeping the overall product design project in mind. Most importantly, it ismultidisciplinary with the chemical engineer having a deep appreciation of issuesoutside of the traditional chemical engineering discipline. This allows the chemicalengineer to drive the product design project in collaboration with personnel inmarketing, finance, business development, chemistry, physics, mechanicalengineering, electronic engineers, and so on. In this framework, the many productdesign and development tasks can be classified into management, sales andmarketing, research and design, manufacturing, and finance and economics. Theseare performed in three phases – product conceptualization, product design andprototyping, and product manufacturing and launch. The framework includes rule-basedmethods such as Quality Function Deployment and the RAT2IO module, and model-based methods such ascomputer-aided molecular design, and transport models. It also includes databasesfor chemicals and equipment, and computer-aided tools for property prediction,process simulation, molecular design, computational fluid dynamics, etc. Thisframework will be illustrated with examples involving solar cells, creams andpastes, LED lamp, smart windows, batteries, etc.

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Recent Advances in Mathematical Programming Techniques for the Optimization of Process Systems under Uncertainty

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Optimization under uncertainty has been an active and challenging area of research for many years. However, its application in Process Synthesis has faced a number of important barriers that have prevented its effective application. Barriers include availability of information on the uncertainty of the data (ad-hoc or historical), determination of the nature of the uncertainties (exogenous vs. endogenous), selection of an appropriate strategy for hedging against uncertainty (robust optimization vs. stochastic programming), handling of nonlinearities (most work addresses linear problems), large computational expense (orders of magnitude larger than deterministic models), and difficulty in the interpretation of the results by non-expert users. In this paper, we describe recent advances that address some of these barriers. We first describe the basic concepts of robust optimization [1], including the robust counterpart, showing its connections with semi-infinite programming. We next consider two-stage and multi-stage stochastic programming in the case of exogenous parameters [2], for which we describe acceleration techniques for Benders decomposition, hybrid sub-gradient/cutting plane methods for Lagrangean decomposition, and sampling techniques. We then address the generalization to the case of both exogenous and endogenous parameters [3], which gives rise to conditional scenario trees for which theoretical properties are described to reduce the problem size. To avoid ad-hoc approaches for setting up the data for these problems, we describe approaches for handling of historical data for generating scenario trees [4]. Finally, we illustrate the application of each of these formulations in demand-side management optimization, chemical supply chains under disruptions, planning of oil and gas fields, and optimization of process networks, all of them under some type of uncertainty.

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Keynote

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Supply Chain Simulation: Creating Competitive Advantage for DSM

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Supply Chain Management and Research are rarely combined in industry. In this presentation we will show that when they are, significant benefits can be obtained. The strategic choices made in supply chain management (SCM) have great impact on cost, inventory and customer service experience warranting a clear effective and optimal strategy and operation. DSM and the markets it operates in are continuously changing, thereby creating increasingly complex and dynamic supply chains. A trend which requires periodic re-evaluation of the supply chain strategy.

DSM combines extensive supply chain (design) experience with simulation and optimization. We employ a broad supply chain optimization toolset, consisting of modular blocks for advanced forecasting, production-, inventory- and network optimization. All tools can be combined with each other and with the two overarching modules; optimization and sensitivity analysis.

Advanced forecasting turns public and private DSM data into quantitative indicators for market price and volume. We will show evaluation and validation of existing methods for use in our markets, proving their value for use in our industry.

Production optimization is used to optimize supply chain cost for operations. Modeling the production process in timing and capacity enables balancing of asset utilization, production cost inventory and customer delivery reliability. We will show how DSM has developed a method for fast and largely automated model development, based on existing discrete event simulation tools.

Network optimization adds the complete warehousing & logistics network to the optimization, determining optimal manufacturing (locations and planning strategy), inventory (locations & target levels) and transport (routing & cost). Initial optimization was and still is being done with existing methods, which after tuning to our supply chains have proven to deliver significant results. Next to this, we will show how DSM implemented tools for multi echelon, multi product, multi asset production allocation optimization with competition for resources.

By being prepared and using a pragmatic approach we were able to establish 10 to 20% increase in perfect order rating, 10 to 20% reduction in supply chain costs and 30 to 50% reduction of inventory at different units over the last 3 years. While at the same time enabling greater competitive advantage by having a more transparent, efficient, flexible and responsive supply chain.

DSM will continue its development of Supply Chain optimization tools to retain our competitive advantage in supply chain operations. Two main research topics for DSM are dynamic market simulation based on agent based modeling and further advancements in market prediction based on available large datasets.

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Processing Pathway/ Supply Chain Optimization Problems for Emerging Energy Technologies: Issues and Some Promising Directions

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Processing pathway / supply chain optimization problems for emerging energy technologies (e.g., renewable energy, carbon capture and utilization) are oftentimes characterized by a large number of technological options, significant amounts of uncertainty, and multi-scale nature of decisions. This presentation examines these characteristics through practical examples and offers some promising research directions. The problem of large number of technological options will be first introduced through the examples of microalgae-based bio-refinery and CO2 capture/conversion. Superstructure based modeling and optimization will be presented as a tool to investigate the problem at a high level in the presence of significant technological and economic uncertainties. Then, the presentation will move onto the issue of coupling between long-term planning decisions like capital investment and policy and shorter-term decisions like production capacity operation and logistics. This aspect manifests itself as a large number of decision variables and constraints complicating solution of the optimization. The optimization complexity gets greatly amplified when the issue of uncertainty is added to the problem. We will examine both two stage and multi-stage problems. Examples of biofuel processing supply chain and energy portfolio optimization for power generation will be used to bring out the essential features and complications. For solutions, stochastic programming and approximate dynamic programming will be introduced.

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PSE Tools for Process Intensification

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In recent years, Process Intensification (PI) has attracted much interest as a potential means of process improvement, to meet the increasing demands for highly efficient processing and for a sustainable production. 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. 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. Hence, it is believed that tools from Process Systems Engineering are keys to enable the implementation of PI in industry.

As PI can be achieved at different levels mainly the process/plant level, the unit operation / equipment level, functional / phase / phenomena level as well as molecular level, different PSE methods/tools on how to systematically address the identification and benchmarking of PI solutions at different levels exist. Each of those has its advantages and disadvantages. Process synthesis tools at higher levels allow the potentially quick identification of a set of suitable PI equipment to improve the process but are limited to the initial search space of PI solutions. Process synthesis tools for PI at lower levels may allow the generation of PI solutions which have not been identified and assembled as equipment before but the problem to be solved is much more complex.

Representing a set of developed PSE tools to assist the selection of the best way to intensify a process, the development of a general systematic PI synthesis/design methodology with an efficient solution procedure of the mathematical synthesis problem, based on the decomposition approach will be presented in detail. Starting from an analysis of the problem definition, 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 at different levels 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. For example, PI unit-operations are stored and retrieved from a knowledge-base tool while phenomena are stored and retrieved from a phenomena library. The methodology will be presented and highlighted through the application to case studies.

[71]

Advances in Chemical Reaction Analysis and Optimization

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The first step after the chemist conceptualizes a new reaction route is experimentation. Experimental results often show undesirable by-products or poor reaction performance. In the process of evaluating the potential to improve reaction performance, several questions need to be answered, such as:

- What is the most probable reaction mechanism and kinetics?
- How should the next experiments be designed?
- What is the best performance that can be achieved for this reaction route?

Answering these questions systematically can be time consuming. The challenges here come from the need to analyze a large number of candidate mechanisms and kinetic models and also the complexity of formulating and solving the mathematical models for kinetic estimation and reactor optimization. In industrial settings, these time intensive tasks may not always fit within the timeline to bring the product to market. Our work has focused on developing a methodology and software infrastructure (REX) to make these tasks significantly easier to execute and thus speed up the mechanism discovery and reactor optimization tasks.

The infrastructure we have developed contains both the knowledge management and project execution components. A reaction library stores the reactions and the associated kinetics which can be centrally accessed. For project execution, the reaction engineer starts with the hypothesis of the reaction mechanism and the available experimental data to develop the most likely kinetic model. Once the kinetic model is developed, simulation and optimization studies can be performed to find the maximum potential for reaction performance. Ease of use ensures that the software allows chemists and engineers to focus more on improving reaction performance rather than burdening them with the intricacies of building and solving the differential algebraic optimization models that are common for these systems.

We will present case studies ranging from monomers, polymers and fine chemicals that illustrate our methodology and highlight the results in improving reaction performance.

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Towards the integration of process design, control and scheduling: Are we getting closer?

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The integration of design and control, control and scheduling and design, control and scheduling, all have been core PSE challenges. While significant progress has been achieved over the years, it is fair to say that at the moment there is no a generally accepted methodology and/or 'protocol' for such an integration - it is also interesting to note that currently, there is not a commercially available software [or even in a prototype form] system to fully support such an activity.

Here, we present the foundations for such an integrated framework and especially a software platform that enables such integration based on research developments over the last twenty-five years. In particular, we describe PAROC, a prototype software system which allows for the representation, modelling and solution of integrated design, scheduling and control problems. Its main features include: (i) a high-fidelity dynamic model representation, also involving global sensitivity analysis, parameter estimation and mixed integer dynamic optimization capabilities; (ii) a suite/toolbox of model approximation methods; (iii) a host of multi-parametric programming solvers for mixed continuous/integer problems; (iv) a state-space modelling representation capability for scheduling and control problems; and (v) an advanced control toolkit for multi-parametric/explicit Model Predictive Control and moving horizon reactive scheduling problems. Algorithms that enable the integration capabilities of the systems for design, scheduling and control are presented along with applications in sustainable energy systems, smart manufacturing and personalized healthcare engineering.

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Industrial Reflections on Modelling of Fine Chemicals and Seeds Process/Product Design

Patrick M. Piccione

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Chemical engineering relies heavily on numerical, quantitative descriptions of physical and chemical processes. With the advent of modern hardware, all practising engineers have at their disposal computational power undreamed of half a century ago. Although software improvements have followed a similar trend, the expectations in terms of quality (cost, speed and accuracy of predictions, etc.) of process development have followed suit as well.

Typical scientific problems addressed through modelling are exemplified within the agri-business company employing the author. Successes and limitations of various approaches are pinpointed through the lens of various application areas. Problems deserving further study are also delineated, as a challenge and opportunity to the modelling community. Implementation and education perspectives conclude these reflections.

Modelling remains not only a critical enabler in the scientific workflow, but also an active, fertile area of research.

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Chemical Production Scheduling: From Models to Online Solution Methods

Christos Maravelias

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We present an overview of recent advances in chemical production scheduling, including a general framework, new modeling and solution methods, and some concepts for the online solution of scheduling problems. First, we develop a framework for the description of scheduling problems in the chemical industries. While building upon ideas used in discrete manufacturing, the proposed framework accounts for features such as material handling restrictions which make chemical production environments different. Second, we present a classification of the various modeling approaches that have been presented in the process systems engineering (PSE) literature and offer some critical insights. Third, we briefly review a series of mixed-integer programming (MIP) models we have developed to address limitations of existing approaches. Fourth, we present an overview of two solution methods that lead to order-of-magnitude speedups, namely, a constraint propagation algorithm for the calculation of parameters used to generate tightening constraints, and a series of reformulations. Fifth, we present a state-space formulation for general scheduling problems. We discuss the modeling of "scheduling disturbances", as well as stability and recursive feasibility in the context of scheduling. We close with some thoughts on the treatment of scheduling as an online problem with desired closed-loop properties.

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Incorporating Process Synthesis in the Processing Systems Design Course

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In the United States, design and analysis of processing systems is often the capstone course integrating many components of the chemical engineering curriculum into a design experience. Chemical process design, plant design, and sometimes even product design are used as example systems domains. Design elements generally include steady-state process simulation, equipment specification, economic analysis, and sometimes elementary optimization, scheduling, and plant-wide control. At both Purdue and Carnegie Mellon we also include significant instruction in synthesis, or the generation of design alternatives. Process synthesis approaches include evolutionary modification, systematic generation, and superstructure optimization. Application areas covered in the courses include reaction path synthesis, species allocation (input-output-recycle-contaminant removal structure), chemical and physical processing task identification, task integrations including energy and power recovery, separations scheme sequencing, heat-integrated distillation, exploitation of nonideal solution thermodynamics, process intensification, and other process synthesis subjects. Strategies for incorporating synthesis concepts into the design course will be described.

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Industrially Applied PSE for Problem Solving Excellence

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PSE, process systems engineering, is about the development and application of systematic methods to process engineering. By means of software tools, the application of these methods is facilitated. Since about half a century, CAPE (computer aided process engineering) tools have found their way in process engineering. E.g. nowadays it is unthinkable to design a plant without a simulation in a flow-sheet package. But there are many more applications of PSE in industry. In this presentation we would like to give a flavor of the type of PSE activities we employ in our company and the kind of CAPE tools we use.

The typical engineering work stream comprises of the development of (conceptual) process design, mass and energy balances, equipment selection and sizing, control strategies, techno-economic evaluations and so on. CAPE tools are applied in all of these work streams.

In process R&D, PSE offers a structured framework for the development of novel processes or optimization of existing ones. Obviously, CAPE tools offer an elegant way for early techno-economic evaluation of conceptual designs. Some of the CAPE tools, which have demonstrated their usefulness in process design, can also be applied in product design.

But it is particularly useful to applying the basic principle of PSE in process development work or plant troubleshooting. In process development, the systematic engineering approach of PSE guides the laboratory experiments, it helps in interpreting the experimental observations and it assists in translating the results to other process configurations and conditions. In plant troubleshooting it offers a systematic and structured way by reducing the complexity of the plant.

Therefore PSE is more than just CAPE by offering a systematic and structured framework. Using principles of PSE, we strive for the best of the worlds, combining experimental or plant observations and computer simulations. In this way, PSE enhances our problem solving excellence.

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Modeling in Process Industry: Needs, Applications and Challenges

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Since many years CAPE software plays an important role in operation and design of chemical processes of all kind. Nevertheless there is still considerable motion in this field. New tools come up, new methods and techniques are developed in industry and university. On the other hand daily practice in industry is mostly lagging behind the state of the art. The reasons for this are:

- Missing knowledge about physical properties and reaction kinetics
- Problems in bringing new methods together with standard modeling tools
- Lack of time for implementing new methods and tools

Within Bayer Technology Services standard CAPE applications are:

- Mass and energy balances for large complete plants
- Operator training systems for startup and operation
- Monitoring tools for plant support and trouble shooting -
- Design of equipment (Reactors, Heat-Exchangers, Distillation Columns)

These issues form 80% of the daily work and are covered by the usual “workhorses” in CAPE technology. As a new trend, the integration of Computational Fluid Dynamics, Thermodynamics and Reaction Kinetics is coming up, but still suffering from restrictions in theory and computational power. The most painful gaps and challenges exist in the following fields:

- Holistic modeling of hybrid (batch/conti) processes
- Rigorous optimization using standard modeling tools
- Complex data analysis to correlate actual problems in the plant with dynamic phases like startup or shutdown from the past

More on the organizational side we have considerable problems to guarantee continuity and conservation of know how in times of high fluctuation of human resources.

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Sustainable Production of Liquid Fuels

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Renewable energy sources are currently being looked at as an alternative to the usage of fossil fuels. The U.S. Energy Information Administration projects a 5% decline in the use of petroleum and other liquid fuels for energy consumption by the year 2040, allowing for the growth of alternative liquid fuels [1]. One possible source of renewable liquid fuels is in the form of biologically derived biofuels, such as bioethanol. Biochemical processes designed to produce these biofuels have the advantage of utilizing many different biomass feed stocks, such as agricultural residues, forestry residues and energy crops, and conversion technologies. The investigation of these process options can determine an economically viable alternative to the current dependence on fossil fuels.

Current studies on the optimization of a separate hydrolysis and fermentation (SHF) process involving the conversion of multiple possible feed stocks using various possible conversion technologies show ethanol (EtOH) can be made in an economically viable matter. The biological conversion of biomass to EtOH in SHF involves four process steps: pretreatment of the biomass to break down the lignin and allow access to the sugars polymers, hydrolysis of the polymers into monomer sugars, anaerobic fermentation of these sugars to the ethanol product, and separation of the resulting EtOH to a pure form. Results from this study show that approximately 76 million gallons of EtOH can be made using a feed of sugarcane bagasse pretreated with sodium hydroxide. The minimum EtOH selling price (MESP) is $2.75 per gallon.

While the results of the SHF study are promising, steps can be taken to improve the MESP. 67% of the MESP is a result of energy and waste treatment needs of the process. Energy integration would allow for a further decrease of MESP through the decrease of these large costs. The waste water stream of the process has large amounts of lignin and other sugars remaining from the ethanol conversion. Energy production via steam generation through the separation and burning of these residues will be investigated, hypothesized to cause a decrease in both the energy and waste treatment needs of the SHF process and reducing the MESP.

Additionally, consolidated bioprocessing (CBP) is a technology that replaces the separate hydrolysis and fermentation with a single organism capable of both functions, removing the need for enzyme addition, and shows promise for an even more economical plant design [2,3]. CBP has the potential to surpass the economic potential of SHF process technologies. This alternative process design will be investigated by finding the optimal design of a bioethanol CBP plant with various biomass feed stock options and corresponding pretreatment technologies. A global sensitivity analysis of both the SHF and CBP processes will be conducted and the processes will be compared to determine which provides the most economical design for the production of bioethanol.

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Steam System Optimization at Mitsubishi Chemical Corporation Kashima Site

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Mitsubishi Chemical Corporation Kashima Site is purchasing steam and power from Kashima-Kita Electric Power Corporation, which is the main distributor of steam and power in Kashima Industrial Area.

Operators in Kashima Site was trying to minimize steam purchasing cost by adjusting the balance of steam production and consumption especially at the second ethylene plant. However, due to possibility of many different operating patterns of the plant, it was difficult for operators to find and keep the optimum steam balance all the time.

Therefore, we have prepared a complete steam system model of the overall factory, and with this model, an optimization system which determines the optimum operating pattern of the plant from 800 thousand possible operating patterns has been developed. The system has also been provided with web-based visualization tools for monitoring of the optimized condition of the plant. Furthermore, the system has been integrated with the advanced process control system to realize automatic adjustment of the optimum operating condition of the plant. The annual benefit of the application of the system in 2012 has been estimated as 50 million yen (500 thousand US dollars).

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Control of Reaction Systems via Rate Estimation and Feedback Linearization

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Model identification and controller design are often seen as closely related tasks, since the control law is calculated using the plant model. Previous control approaches based on extensive variables or inventories are examples of this strong dependence on the model [1, 2]. Since the identification of chemical reaction systems can be a time-consuming and complex task, one would ideally like to avoid it as much as possible. The concept of variant and invariant states allows isolating the different rates in chemical reaction systems, thereby facilitating analysis, monitoring and control [3-5]. Using this concept, one can estimate dynamic effects without the need of identifying the corresponding kinetic models.

This contribution presents a feedback linearization approach that is based on the estimation of unknown rates, such as the rates of reaction and mass transfer, thus allowing efficient control without the use of kinetic models.

Rate estimation uses the numerical differentiation of appropriately transformed extensive variables called rate variants that are invariant with respect to the manipulated variables. A rate variant contains all the information about the corresponding rate and, as such, is decoupled from the other unknown rates. Since it is possible to estimate the unknown rates this way, the controller does not require kinetic information. However, because of the differentiation step, the controller is most effective with frequent and precise measurements of several output variables.

Feedback linearization sets a rate of variation for the controlled variables, thereby guaranteeing quick convergence of these variables to their set points. For open chemical reactors, the parameters of the feedback linearization controller are determined by readily available information, such as the reaction stoichiometry, the heats of reaction, the inlet composition or the inlet and outlet flow rates. This novel control strategy is illustrated in simulation for the control of both concentration and temperature in a continuous stirred-tank reactor.

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[190]

New paradigm of chemical process design: from molecule to system

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Chemical process design is central to chemical engineering, which starts at a conceptual level and ultimately ends in the form of constructed plans. In general, chemcial process design relies on simulation based on mathematical equations which are formed according to the principles of thermodynamics, kinetics, transfer properties and so on. Generally a chemical process consists of multi scales, i.e., molecule, fluid/solvent, unit and process, which causes process design involving multi disciplines, thus the new breakthroughs, discoveries, viewpoints of other disciplines would certainly bring about both possibilities and necessities to develop new methodology and upgrade the knowledge system of chemical process design.

For a real chemical process, related phenomena covers a broad range both in spatial dimension and temporal dimension which extends from the molecular to the plant scale. Thus, multi-scale method for process design, especially the scale-bridging, becomes more and more important. The benefit of integrating the molecular information into process design will shrink the R&D period, and provide useful information to guide the lab and pilot plant studies. However, this also poses many scientifically challenging problems.

In this study, the multi-scale simulation and integration methodology is proposed, and ionic liquid-based process design for gas separation is conducted as a case study, which focused on the following aspects: 1) Quantum-chemical (QC) simulations are firstly carried out to investigate the relationship between the structure and the properties of ionic liquids (ILs), then determine the key factors that will improve the solubility and selectivity of the ionic liquids to gases involved. The interaction force between the gas and IL is studied to understand the separation mechanism and design promising ILs; 2) new thermodynamic models of the ionic fragment contribution-corresponding states (FCCS) are developed to predict the physicochemical properties of ILs and phase equilibrium of IL-containing mixture systems. The contribution values of ionic fragment are estimated by QC method, which means the influence of molecular structure on macro properties could be discovered; 3) the bubble behavior, such as bubble size distribution, gas holdup, Sauter diameter are studied, and then the fluid dynamic and mass transfer properties are modeled and predicted; 4) with these parameters, process simulation was performed with a commercial simulator to determine the operating parameters and the flowsheet structure considering real industrial constraints; 5) techno-economic performance and environmental impacts are assessed on the basis of the above information, and the multi-objective method is conducted to optimize key parameters both in the molecular level and process level with the aim of minimizing the energy demand, the cost and environmental impact for gas processing with ionic liquids.

Based on the above framework, several task-specific ILs and related processes are designed and optimized for CO2 capture, SO2 capture and NH3 recovery. The results will also be verified by subsequent lab experiment and pilot plant.

[244]

Industrial perspectives on deployment of scheduling solutions

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Despite many significant achievements in the development of scheduling methods and solutions one important still unresolved technical challenge and hurdle is their deployment in an industrial context. Today, the most typical and successful approach to bring a theoretical solution “live” is that plant experts directly collaborate with the university experts to locally build a solution that is tailored to their needs. This often results in strongly tailored implementations that are normally not reusable, which limits a wider distribution of novel approaches. Also, unlike for hardware solutions (e.g. PID-controllers), the lifecycle of the locally developed scheduling solution heavily depends on the availability of the key implementers on-site and the long-term strategic interest and commitment of the company management to maintain and further enhance the tools. However, here it should be mentioned that a multitude of scheduling companies are successfully extending their businesses mainly based on already established technologies. This means that in times where cost- and process efficiency or throughput is valued higher than ever it is not evident how novel optimization strategies can reach their end users.

The need for new optimization schemes is growing as they have been also addressed by the earlier PSE-events (2009; 2012). With the ever increasing availability of data and higher level of automation and electrification production scheduling cannot anymore be seen as an autonomous solution. Concepts such as Internet-of-Things, Smart Grids, Smart Manufacturing, Industry 4.0 and enlarged scope on Enterprise-wide Optimization topics (2012) increase the pressure to connect and interact with neighboring solutions and systems. Examples of this are the increasing research on industrial Demand-side Management (e.g. 2014) taking advantage of the fluctuating price information of electricity, as well as integration of scheduling and control (e.g. 2012; 2012) ensuring, among others, that the provided schedule is also aware of the underlying process. In an industrial environment, a scheduling solution cannot live as an “island” but must be closely connected to the production environment (often a DCS, MES or CPM system) in order to be able to automatically obtain all the production and process data that is important for scheduling. In a similar fashion, integration to the supply chain (ERP) level (2009) is important in order to receive up-to-date order situation, including their priorities.

The new scheme does not only challenge the solution algorithmic developers – mostly Academia – through the ever increasing problem sizes, faster solution response times, modeling challenges when combining various domains into one concept and higher expectations on solution quality, but also requires a significant improvement in deployment efficiency in the industries (2014). Here the key challenges are to create more modular and flexible systems that enable seamless data communication and even can combine earlier separated business models. Standards such as ISA-95 (2005) can be helpful in paving the way for some of these mandatory tasks. In this paper we discuss some of the hurdles for deploying scheduling solutions with concrete examples of integration schemes benefitting from standards. Some needs for improvements are identified both in Academia and Industry, as well as the fact that the two communities can be aligned much better than has been achieved so far.

[257]

The role of Process Systems Engineers on designing sustainable products and processes

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The aim of this talk is be to cover the role of process systems engineers in the design, scale up and development of new products and processes that are of the right quality and sustainable. It will intend to cover major aspects that need to be taken into account to successfully embed quality and sustainability concepts during product and processes development. Finally, it will cover some of the key capabilities that process system engineers need to foster and enhance to prepare for the future challenges in designing products and processes.

[448]

Abnormal situation management challenges and opportunities in the big data era

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The modern chemical plants are often equipped with advanced protection systems such as automatic control systems, alarm systems and emergency shutdown systems for quality and safety assurance. However, unplanned shutdowns that are caused by abnormal situations still happen with an unsatisfactorily high frequency, which leads to huge economic losses and unpleasant environmental emissions. In an extreme situation when the advanced protection systems fail, major chemical accidents may occur, which generally lead to disasters such as the BP Texas city refinery explosion accident in 2005. To disclose the root causes of these adverse consequences, the shortcomings of the advanced protection systems are analyzed in this paper. To complement the weakness of the advanced protection systems, abnormal situation management (ASM) has been proposed for about two decades. Tremendous efforts have been made to develop various ASM technologies. However, the implementation of those technologies in the real industrial world is not satisfactory. Challenges that ASM faces are described in this paper. With the rapid information technology advancement, nowadays a big chemical corporation is standing inside a big data environment which has drawn great attentions. How to efficiently utilize the big data for improving quality, health, safety and environment (QHSE) has become a very hot research frontier. Smart manufacturing is one of those concepts that were proposed recently. One of the key to smart manufacturing is how to increase the risk awareness in the whole chemical manufacturing facility. Opportunities for ASM therefore arise. The ASM technologies developed by the author's research are introduced in this paper with a real industrial application case study in a big data environment of a large petrochemical company.

[473]

Overview of Smart Factory Studies in Petrochemical Industry

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The smart plant in petrochemical industry is operational excellence as the goal, through the operational management of the whole process, with a high degree of automation, digitization, visualization, modeling and integrated refining chemical plant, which is the future development direction of the petrochemical enterprises. This paper discusses the development process of petrochemical industry smart plant, describes its architecture, key technologies and applications. Then based on industry background, the paper gives a smart factory model definition. It puts forward thesis in production control, equipment management, HSE management, energy management, supply chain management and decision support six business domain as the focus, information technology and standardization to support the petrochemical smart plant "6+2" model framework. Finally, the paper points out the future development trend of smart plant and further research directions.

[479]

Cognitive Engineering: Towards Preventing Human Error during Process Operations by Real-Time Monitoring of the Plant Operator

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Process industries continue to suffer from accidents despite significant regulatory intervention since the mid-1980s and major developments in process control, monitoring and supervision technologies over the last four decades. Human error is widely agreed to be the major contributor to most accidents today. The traditional approach has been to look at human error as the initiating event of incidents, one that has a given likelihood of occurrence, similar to the way that a piece of hardware is expected to fail at some frequency. Just like equipment monitoring relies on detecting prognostic signatures of its impending failure, well in advance of the actual occurrence so as to trigger timely intervention, one can ask, is it possible to detect human error before it is committed? In this paper, we will explore if this "Minority Report" type technology is now within the realms of reality, at least in the limited context of DCS operators.

Cognitive engineering is concerned with the mental processes of the human actor, such as perception, memory, reasoning, and motor response especially in the context of his/her interactions with other elements of a system. In this talk, I will provide an overview of recent developments from this emerging field such as eye gaze tracking and pupilometry, which offer real-time measurements of the operators cognitive state. I will demonstrate using results from recent experimental studies at IIT Gandhinagar that these measurements contain signatures indicative of various levels operator's situation awareness. When the operator's situation awareness levels becomes low, operators are highly likely to take incorrect control actions and trigger a chain of events with the potential to cause incidents and accidents. Finally, I will also describe a number of potential applications of these operator monitoring technologies, ranging from process design to control and operator training.

[493]

Process Systems Engineering Approaches to Multi-Scale Chemical Product Design

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Product design problems by nature are open ended and may yield many solutions that are attractive and near optimal. An additional complicating reality is that properties of materials are controlled by a multitude of separate and often competing mechanisms/phenomena that operate over a wide range of length and time scales. This presentation will highlight several novel methods for chemical product design, including: 1) Ionic liquid design by multivariate characterization; 2) Spatial molecular signature descriptors for generation of non-peptide mimetics; and 3) Modeling the dispersability of polydisperse nanoparticles in gas-expanded liquids.

A characterization based group contribution method (cGCM) has been developed from infrared (IR) spectra of a representative training set of ionic liquids (IL) that contain large quantities of descriptor information on molecular architecture. The spectra are generated using density function theory (DFT), which make the characterization techniques independent of the availability of experimental spectroscopic data. To identify systematic patterns and important features of the molecular architecture in such multivariate data, multivariate statistical techniques such as principal component analysis (PCA) and partial least square (PLS) are used. The reverse design of potential IL molecules is accomplished by exhaustively generating combinatorial structures from the set of basic groups, which represent the chemical make-up of the training set fragments, until the resulting properties match the target property values.

A novel method for incorporating three-dimensional structural information in molecular design algorithms has been developed. The molecular signature descriptor provides a systematic way to encode the atom type and connectivity of a molecular structure, where the signature of a molecule is a linear combination of its atomic signatures. We have recently extended this method to include three-dimensional information in the form of a spatial molecular geometry matrix, which can be manipulated to provide several useful descriptors. The ability to include the spatial/topographical (3D) arrangements of the atoms in a molecule is particularly important in applications such as molecular recognition.

Due to the size-dependent properties of nanoparticles it is often necessary to fine-tune the materials for their intended application, e.g. contrast agents in medical imaging, drug delivery vehicles, highly selective catalysts, etc. A thermodynamic model has been developed that can accurately predict (typically within 5%) the average size and size distribution of size-selectively fractionated nanoparticles. The application of the model is demonstrated using experimental data for a system of dodecanethiol-stabilized gold nanoparticles in hexane that are precipitated by the addition of CO_2.

[631]

A PSE approach to patient-individualized physiologically based pharmacokinetic modeling

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Pharmacokinetic modeling allows predicting the drug concentration reached in the blood as a consequence of a specific administration. When such models are based on mammalian anatomy and physiology it is possible to theoretically evaluate the drug concentration in every organ and tissue of the body. This is the case of the so-called physiologically based pharmacokinetic (PBPK) models. This paper proposes and validates a procedure to deploy PBPK models based on a simplified, although highly consistent with human anatomy and physiology, approach. The article aims at reducing the pharmacokinetic variations among subjects due to inter-individual variability, by applying a strategy to individualize some model parameters. The simulation results are validated respect to experimental data on remifentanil.

[646]

Modeling and Optimization of Continuous Pharmaceutical Manufacturing Processes

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The increased availability of software tools for solids-based process modeling has created opportunities to enhance pharmaceutical development through the use of models. In particular, recent work in the area of integrated process modeling has demonstrated the potential of these simulations to complement experimental studies during process development. Once developed, these models also facilitate the use of other mathematical tools like process feasibility analysis and optimization. This work will emphasize recent developments in the area of flowsheet modeling for pharmaceutical processes. Methods for feasibility analysis and optimization of these complex process models will also be discussed. These tools can play an important role in pharmaceutical process development.

[657]

Modeling the Fixed-Bed Fischer-Tropsch Reactor in Different Reaction Media

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Reactor modelling is a very useful tool in the design and scale-up of commercial reactors, enabling prediction of the system behaviour under different operating conditions without the need for expensive and time-consuming experimentation. In this paper we present our approach towards developing a comprehensive fixed-bed reactor model for Fischer-Tropsch synthesis (FTS) over a cobalt-based catalyst using a detailed mechanistic model to predict the FTS hydrocarbon product distribution. FTS is the heart of the X-to-Liquid (XTL) technology as it is the process by which synthesis gas (a mixture of carbon monoxide and hydrogen obtained from natural gas, coal or biomass) is converted into ultra-clean fuels and value added chemicals. In the current study, we have developed a MATLAB® code that uses a Genetic Algorithm technique to estimate the parameters of detailed mechanistic kinetic models, taken from the literature, which are based on well-known mechanisms such as the carbide and CO-insertion mechanisms. Simultaneously, we have implemented a fixed-bed reactor model, also in MATLAB® that is capable of predicting the whole bed behaviour taking into account the heat and mass transfer resistances in the reactor bed such as the loss in catalytic activity due to diffusion in the catalyst pores. For experimental validation of the model, a high pressure bench-scale reactor unit has been commissioned to conduct FT experiments in different media such the gas-phase (which is the current commercial standard) and supercritical solvent phase (which has been shown on the lab-scale to have certain advantages over conventional gas-phase operation). Using our reactor unit, we have obtained the detailed product distribution and the rates of formation of paraffins and olefins from a set of FTS experimental data carried out under gas phase conditions at low syngas conversion. These data have been used as input for the Genetic Algorithm code in order to fit the parameters for the different kinetic models. At a later stage, we intend to conduct experiments in the supercritical hexane solvent phase. Data generated from these experiments will be used to give insight into the mechanism of FTS in the presence of a supercritical solvent. The results of these studies could enable us to suggest modifications in existing kinetic models thereby accounting for the effect of the supercritical solvent on the system. The kinetic model developed here is to be integrated into a model of the whole reactor bed, with a view towards facilitating the optimization and scale-up of novel FTS reactor bed designs.

[776]

Advanced Chemical Manufacturing and Sustainability: A Multidisciplinary Collaboration Approach

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Global manufacturing competition has begun to shift towards advanced material-product-process design, fast implementation, just-in-time model-based manufacturing, frequent product transitions, and shifting of technical personnel to meet those changing needs. The fundamental principle in these endeavors is the assurance of engineering sustainability. In the U.S. academia, engineering sustainability, advanced manufacturing theory, alternative energy and biofuels, and advanced nano and biotechnologies, have become very active but relatively disconnected research areas. Research coordination in the academic community and its networking with industries are insufficient and lack depth. To bridge the gap between the academic knowledge discovery and industrial technology innovation for sustainable manufacturing, a multidisciplinary team in the U.S. has created an interdisciplinary, international research coordination network to promote Sustainable Manufacturing Advances in Research and Technology (SMART). This network has a participation of 21 academic institutions from the U.S. and seven other countries, and has an involvement of 11 U.S. national organizations and university research centers.

SMART reflects the theme of the joint effort among a number of leading academic laboratories, centers, non-government organizations, and major manufacturing industries. In the past two years, the multidisciplinary team has worked closely to: (1) conduct comprehensive and in-depth review of frontier research and technological development for sustainable manufacturing, (2) define the roadmap towards manufacturing sustainability and identify the bottlenecks in a number of focused research areas via several workshops, (3) coordinate research through sharing knowledge, resources, software, and results, (4) establish partnerships with industrial groups to expedite technology introduction, and (5) conduct education and outreach to a wide range of stakeholders. Sustainable manufacturing research involves a wide spectrum of areas and disciplines, such as advanced manufacturing, sustainability assessment and decision making, product and process systems engineering, energy and environmental engineering, multiscale complex systems science and engineering, information technology, economics and sociology. The SMART CN has been collaborating towards creation of a new paradigm for manufacturing sustainability, aggregating concerted efforts from multiple research groups with complementary expertise to transform the knowledge base of manufacturing sustainability, and developing a consensus roadmap for future efforts. It is anticipated that success in this endeavor will have a significant impact on industrial efforts in developing sustainable manufacturing technologies. The project is also generating a number of educational modules for sustainable engineering education that should be widely adoptable for undergraduate/graduate education and professional training in industries. This presentation will also highlight 10 research and technology development themes that were identified by a group of leading academic researchers and industrial leaders during a sustainable manufacturing roadmap workshop in 2013.

[950]

Enterprise Risk Management in Complex Socio-Technical Systems: Challenges and Opportunities

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Recent systemic failures in many different domains such as the BP Deepwater Horizon oil spill, and the Subprime financial crisis have reminded us, once again, of the fragility of complex systems. Although the failures occurred in very different domains there are, however, certain common underlying mechanisms driving such systemic failures. Understanding them is essential to avoid such disasters in the future. To understand and learn from them, one needs to go beyond analyzing them as independent one-off accidents, and examine them in the broader perspective of the potential fragility of all complex systems. Systemic failures typically occur due to potential fragility in complex systems. It is their scale, nonlinearities, inter-connectedness, and interactions with humans and the environment that can make these systems-of-systems fragile, when the cumulative effects of multiple abnormalities can propagate in numerous ways to cause systemic failures. In particular, the nonlinear interactions among a large number of inter-dependent components, and the environment, can lead to "emergent" behavior – i.e. the behavior of the whole is more than the sum of its parts, that can be difficult to anticipate and control.

One needs to study all these disasters from a common systems engineering perspective, so that one can thoroughly understand the commonalities as well as the differences, in order to better design and manage such systems in the future. Further, such studies need to be carried out in concert with public policy and regulatory experts (and governmental agencies) so that all the scientific and engineering lessons get translated into effective policies and regulations.

In this talk, I will present an overview of the challenges and opportunities for us in this important area. In particular, I will highlight a novel control-theoretic framework that unifies the social and the technical components of a complex system to better model, control, and manage enterprise risk.

[954]

Process Technology Licensing: An Interface of Engineering and Business

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New technologies are developed at a high rate in many areas like in process industries. Basis for new technologies are inventions and innovations generating intellectual property rights. By licensing, permission is granted to others to use these rights under controlled circumstances. Technology licensing often includes not only patents but for example also know-how, design and trademarks.

Drivers for in- or out-licensing of process technologies are manifold. Some very important drivers are, reducing own development risks, speeding up commercialization, earning money from royalties or partnering with other companies, all of which are business reasons. Engineering know-how of the in-licensing party is necessary to assess the technology, the own development options, the fit within the companies' value chain, and foremost, to calculate the cost benefit using a new process technology. Relevant engineering know-how of the out-licensing party is in offering and selling the technology: Engineers need to describe the advantages for licensees, design and optimize the process, or calculate potential license fees by analyzing the benefits of the technology for the licensee.

The licensing business requires continuous development of the licensed technology. Processes need to be analyzed and continuously improved. Specific and optimized designs for licensees are required based on the licensee's design or optimization targets and constraints. Examples from ongoing business will be used to describe the engineering-business-interface.

[958]

Challenges and opportunities in API process development

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The last few years we have seen a significant transformation in organic chemistry laboratories of pharmaceutical API development. This had lead to the availability of a lot of high quality data, for example utilization of spectroscopic techniques for reaction monitor is now routine. Although the amount of information available has increase dramatically that has not yet translated to a proportional decrease in process development time. Utilization of process modeling although it has increased is far away from routine; probably due to the relative small number of chemical engineers in the field. Pharmaceutical process development still remains primarily a experiment driven process. In most of the cases empirical models are utilized to rather map the final design space than help with the speedy development of the process. The large number of compounds in early development stage and their large attrition as they move to late stage of development puts significant pressure in time and resources available for process development. Process System Engineering and computational technique are key in designing efficient experimentation strategies. Such models need to utilize prior information, be fit for purpose but also act as knowledge capture and maintenance mechanism. They need to be flexible enough and evolve following the project in its journey from early to full development.

We will examining some of these opportunities of PSE applications with examples that span both early and late development.

[967]

Simple rules for economic plantwide control

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When designing new-technology based plants process engineers often operate under a strict time schedule and inevitably, the additional time required to devise a control strategy that achieves not only safe and stable operation but also economic- operation using optimization-based/mathematical methodologies, is often not available. One alternative is to employ practical guidelines that lead to a close-to-optimal control structure design, since those are usually easier to understand, thus easier and faster to implement without requiring high expertise. In this work we exemplify the rules that can be used solely based on engineering intuition a from a systematic procedure plantwide control design procedure proposed by Skogestad (2004). We attempt to present the them in an easy-tounderstand fashion and to demonstrate that even though the procedure is based on a combination of heuristics and plant model optimization, it can be used as a supplement to the traditional practical guidelines by suggesting what to control -or what not to- in order to improve the economics of the plant operation. Additionally, we propose a new simple rule that supplements the existing economic controlled variable selection rules, stated as follows: "Do not control an unconstrained controlled variable that reaches a minimum or a maximum at the optimum". We apply the newly suggested and the existing rules to a simple but quite famous reactor-separator-recycle (RSR) plant operation case study and investigate their effectiveness. We successfully demonstrate that using the practical rules from Skogestad's procedure can potentially improve a plant operation even if the process model is not available.

[1014]

Mixed-Integer Fractional Programming: Models, Algorithms, and Applications in Process Operations, Energy Systems, and Sustainability

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A wide range of optimization problems arising in practical applications can be formulated as mixed-integer fractional programming (MIFP) problems, which combine the combinatorial difficulty of optimizing over discrete variable sets with the challenges of handling the non-convex fractional objective function. This talk will explore recent results on the development of tailored global optimization algorithms to address the computational challenge of solving large-scale MIFP problems. These MIFP methods will be illustrated through three applications: (1) function-unit-based life cycle optimization of sustainable product systems and supply chains under sustainability criterions, (2) integrated optimization of production scheduling and process dynamics of continuous multi-grade polymerization reactors, and (3) optimal design and operations of algae processing network for CO_2 capture and utilization. For each application problem, we will discuss the modeling framework, solution algorithms, and computational results.

[1048]

Advances and Challenges in Modelling of Processing of Lipids

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Alfa Laval Copenhagen A/S, Denmark

Unlike the processing of crude and petroleum oils, the lipid processing industry has until recently not taken much advantage of the progress made in property modelling or process - product design over the last few decades. While there are some similarities in the processing of petroleum and lipids, a number of features of both lipids and their processing present sets of new challenges for chemical engineering developments. A brief introduction will be given to the processing of lipids, emphasizing the refining of edible oil. Some examples are provided on advances in both modelling of the lipids properties (pure components, phase equilibria) as well as how such property modelling enables use of standard process simulation programs for design and process optimisation. These advances have for example lead to new insights on optimum withdrawal of valuable components (micronutrients) in byproducts from refining operations.

[1057]

A perspective on PSE in fermentation process development and operation

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Industrial fermentation processes are increasingly popular for the production of bulk and fine chemicals, pharmaceuticals etc. starting from renewable resources. In addition to that, fermentation also plays a prominent role in 2nd generation bioethanol production processes. As a consequence, industrial fermentation processes are considered to form an important technological asset for reducing our future dependence on chemicals and products produced from fossil fuels.

However, despite their increasing popularity, fermentation processes have not yet reached the same maturity as traditional chemical production processes, particularly when it comes to using engineering tools such as mathematical models, process control algorithms and optimization techniques to support the search for improved and more efficient processes.

This perspective starts with a description of some of the most important engineering challenges within industrial fermentation technology: scaling up and scaling down fermentation processes, quantification of the influence of morphology on fermentation broth rheology and mass transfer, efficient data handling, and introducing novel sensors to measure and especially also to control insightful process parameters. The greatest emphasis is on the challenges posed by filamentous fungi, because of their wide applications as cell factories and therefore their relevance in a White Biotechnology context.

Mathematical models can be considered as useful tools for representing available process knowledge, and can therefore be excellent tools to support process development, as will be illustrated with a number of examples. It will be illustrated how multivariate statistical methods can assist with the interpretation of the increasing amount of available process data generated during fermentation processes. Furthermore, Computational Fluid Dynamics (CFD) is introduced as a promising tool that can be used to support the scaling up and scaling down of bioreactors, and for studying mixing and the potential occurrence of gradients in a tank. Finally, the application of tools such as population balance models (BPM) is discussed, with respect to potential future applications of PBM in the fermentation technology area.

[1120]

Sustainable production and consumption: A decision-support framework based on a systems approach to integrating environmental, economic and social aspects of sustainability

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The idea of sustainable production and consumption is becoming a widely-accepted societal goal in many countries. However, its implementation is slow and the world continues to speed down an unsustainable path. One of the difficulties is the sheer complexity of the production systems that would need to be re-engineered in a more sustainable way as well as the number of sustainability constraints that have to be considered and satisfied simultaneously.

This paper argues that bringing about sustainable production and consumption requires a systems approach underpinned by life cycle thinking as well as an integration of economic, environmental and social aspects. A decision-support framework developed for these purposes will be presented and discussed. Taking a systems, life cycle approach, the framework integrates all three sustainability dimensions to aid decision makers in identifying sustainable technologies and consumption patterns. It comprises a range of tools, including scenario analysis, life cycle assessment, life cycle costing, social sustainability assessment, systems optimisation and multi-criteria decision analysis. The framework will be illustrated trough an application to the integrated energy system in the UK, extending to 2070.

[1123]

Structure Based Drug Discovery and Design from Optimization Perspective: Observations, Applications and Results

Metin Turkay

Koc University, Turkey

Drug discovery and design is a complex and very time-consuming process requiring integration of different disciplines including molecular biology, medicine, biochemistry, medicinal chemistry and mathematical sciences. An important development in drug discovery and design has been the use of high throughput screening. Recently, virtual screening has become an important stage for improving the efficiency of drug discovery and design efforts. Virtual screening can be utilized for browsing databases of molecules. Discovery and design of active drugs against the protein of interest in-silico narrows down drug candidate molecules to be tested experimentally resulting in a rational assessment of drug candidates. Although this approach saves from time and expenses, it has two important challenges. The first one is the analysis of results that are obtained from millions of virtual screening experiments. The second challenge is the generation of novel drug candidates that uses the results from the virtual screening and in-vivo experiments. In this talk, we will summarize our observations on the structure based drug discovery and design and discuss our applications on data analysis and lead optimization using optimization models. We will illustrate our approach on several interesting applications and summarize the results.

[1124]

Systematic Design Procedure of Micro Chemical Plants

Shinji Hasebe

Kyoto University, Japan

The design problem of micro chemical plants has different characteristics with that of conventional plants. For example, one of the dominant characteristics of micro devices is large surface-to-volume ratio. To use this feature effectively, the shape of the device must be included in design variables in addition to the size of the device. Usually, the flow rate of a channel is not enough for industrial production. Thus, the numbering up of channels is requested to increase the production rate. As a channel size is very small, it is difficult for micro chemical plants to add new measurement devices after the construction. This fact indicates that the plant structure and the instrumentation and control systems must be designed simultaneously. In this research, a systematic design procedure considering the above points is proposed.

The design problems of micro chemical plants have hierarchy. First, a single channel reactor is used to examine the characteristics of the reaction. Then, the number of channels is increased, and they are assigned in parallel to a plate (internal numbering up) so as to increase the production rate. Here, the shape of a channel and that of the distribution section are treated as design variables. Several shape design methods are explained using examples. The structure optimization problem of the distribution section becomes a synthesis problem which selects the optimal connections of unit structures from the candidates, and it can be formulated as a mixed integer programming problem. If one plate does not have sufficient production rate, they are stacked, and three-dimensional devices are constructed.

In conventional chemical plants, it is possible to add new measurement devices after the construction of the plant. In the micro chemical plant, however, the design and control problems must be considered simultaneously. Some examples of the shape design that possesses less sensibility about the disturbances are explained. The control systems, which are suitable for micro chemical plants, are also explained considering the above feature. The slug flow is an effective scheme for gas-liquid reaction in the micro channel. When the slug lengths are fluctuated, the efficiency of the reaction may deteriorate greatly. For the device consisting of parallel channels, the effective measurement method of slug flow condition is also explained.

If the capacity of one device is still less than the required production rate, that device is assigned in parallel to increase the production rate (external numbering up). The feature of numbering up structure is summarized and the problems arising at the numbering up procedure are discussed. The blockage is one of major troubles to be overcome for realizing long- term operation of micro chemical plants. However, it is hard to install measuring apparatus to every micro-device to detect the blockage. The smart flow distributer that can detect the blockage of one of the parallelized devices is explained, and the operation procedure that the blockage does not affect the flow condition is demonstrated.

[1133]

Challenges and opportunities for process system modelling in the development of new medicines

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Process development of new formulated medicines is concerned with meeting the required critical quality attributes of the product and ensuring product performance. Although models exist for design of unit operations used in pharmaceutical manufacturing processes, the impact on the product performance will typically be confounded across many unit operations. A key challenge is whether we can adopt a process system modelling approach whereby the individual unit operations can be connected together so that a change in materials or, process parameters at any point in the manufacturing process can be related to intermediate and final product attributes. The main limitation to further development of such an approach is our ability to build more mechanistic models that can be predictive of intermediate properties. In particular a significant proportion of pharmaceutical products are based on particulate or solids manufacturing processes in which there is incomplete understanding of the complex phenomena involved and constitutive models to describe the bulk behaviour of particulate formulations are lacking. Opportunities for increasing the application of simulation in pharmaceutical product development and in so doing increasing the speed, resource and material efficiency and overall level of fundamental understanding are discussed.

[1134]

Large-scale Multiphase Models for Pharmaceutical Manufacturing Optimization

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In this talk first a brief introduction to the current state of the pharmaceutical industry, including current the developments and future challenges, is presented. Specifically, the problems associated with the rational development and the production of oral-dosage forms are discussed. Then, the need for the development of robust and reliable multi-scale models is highlighted to replace trial and error and extensive experimentation.

In this context, various modeling approaches are presented, including the discrete element method (DEM), computational fluid dynamics (CFD), the coupling the combination of CFD and DEM as well as molecular simulations. Processes that are highlighted are the coating of tablets, fluid-bed operations, powder mixing and the leaching from packing materials.

In the field of fluid bed modeling we use the Compute Unified Device Architecture (CUDA) technology that – for example – can be used to perform massively-parallel DEM-simulations with several million particles on a single desk-side Graphics Processing Unit (GPU). Fluidized system simulations with up to 30 million particles are perfomed [1].

In addition, our efforts in the in-silico development of coating process in drum coaters are presented. Here we have recently developed new methods for implementing efficient spray detection in DEM simulations [2]. The spray modeling was performed while the main DEM simulation was running and after the simulation using saved data. Lastly, studies of the mixing of granular materials, i.e., powders, and the wetting of such systems are presented as a prerequisite for the first-principles modeling of high-shear granulators [3]. Finally, our recent work in the modeling of granular systems (blending, extrusion) and molecular modeling (leaching) is presented in this talk.

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[1138]

Modeling in API downstream process development

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In the chemical manufacturing of our API's (active pharmaceutical ingredients), downstream processing is often initiated by crystallization, followed by solid-liquid separation and drying of the solid (intermediate) material. Since these unit operations are omnipresent, modeling tools are applied to support process developments and to guarantee successful process introductions.

Ultimately, we aim for a lean study protocol, i.e. a limited set of data-rich experiments, in combination with accurate models to increase our R&D efficiency and process understanding. In order to meet the expectations regarding efficiency and accuracy, we optimized the data collection and we fine-tuned the models where necessary. Based on a few case studies, the outcome and the benefits of this approach will be demonstrated, and the overall trade-off in modeling downstream processes will be highlighted. We will show that an overall optimization of downstream processes can be performed in silico and therefore, laborious trial-and-error optimizations can be avoided and time-to-markets can be shortened.

[1148]

Statistical modelling and in-line near-infrared spectrometry in process development

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The Pharmaceutical industry has started a transformation from simple end-of-line testing and one-factor-at-the-time process development mentality, to utilizing advanced spectroscopic sensors embedded in production equipment and use of mathematical and statistical modelling tools to guide process development and gain enhanced process and material understanding. In this presentation examples of near-infrared spectroscopic sensors attached to moving powder blenders as well as statistical modelling of process and formulation factors will be shown from process development studies of new biopharmaceutical tablets at Novo Nordisk.

[1149]

Crude-oil scheduling technology: moving from simulation to optimization

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Scheduling technology either commercial or homegrown in today's crude-oil refining industries relies on a complex simulation of scenarios where the user is solely responsible for making many different decisions manually in the search for hopefully globally feasible solutions over some limited time-horizon i.e., trial-and-error heuristics. As a normal outcome, schedulers abandon these solutions and then return to their simpler spreadsheet simulators due to: (i) efforts to model and manage the numerous scheduling scenarios, (ii) requirements of updating premises and situations that are constantly changing, and (iii) manual scheduling is very time-consuming work. Moving to solutions based in optimization rather than simulation, the lecture describes the future steps in the refactoring and remaking of Petrobras's scheduling technology (SIPP) considering in separate the graphic user interface (GUI) and data communication developments (non-modeling related), and the modeling and process engineering related in an automated decision-making with built-in problem representation facilities and integrated data handling features among other techniques in a smart scheduling frontline.

[1150]

Economic evaluation of large scale bioprocesses – technical and business issues

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During the last 30 years the pharmaceutical industry has provided a significant number of essential drugs that can only be manufactured using biologically-based production routes, using enzymes or cell cultures: human insulin and other essential proteins, vaccines, in addition to cancer drugs extracted from metabolic pathways.

In contrast, biologically-based routes to commodity chemicals need to compete with classical routes based on intermediates from the petroleum industry. Whereas the position of the bio-industry is dominant within pharmaceutical production, the production of bulk chemicals and intermediates for the polymer industry is still largely based on classical chemical routes. Nevertheless, some large scale bioprocesses, for example to amino acids (lysine), citric acid and antibiotics (penicillin) are undoubtedly successful, and during the last 15 years intermediates for polyesters (1,3 propane diol) and for polylactides have been produced at a scale of 105 ton/year.

However, many more bio-based routes to polymers are in the pipeline, and chemical companies around the world are entering the market. In this lecture we shall outline how a set of decisions has to be made along a 3-5 year time line that may or may not lead ultimately to a large scale, competitive biologically-based route to a given commodity chemical.

Decisions at a fundamental level have to be made in the initial investigation phase: What is the yield of the desired product that can be expected, will there be byproducts, and will the productivity be sufficiently high to compete with conventional production routes?

Subsequently, the downstream process needs to be considered: The producing strain may be modified to allow processing, for example at a lower pH – thereby avoiding byproducts or facilitating capture and purification of the desired product.

Gradually a technically optimal process is built up with due consideration of the need to arrive early in the market. The improved process must be documented at pilot- and demonstration scale, and now a realistic estimate of the viability of the process at large scale can be assessed before a major capital investment is committed.

As a final consideration the market advantage of a sustainable, environmentally friendly bio-process must also be realistically assessed.

[1155]

New Perspecitve of Simulation & Modeling to Accelerate Development of Petrochemical Products

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Developing new products in petrochemical industry typically has a numbers of challenges. One of the key issues is the scaling up from lab to commercial process. Although the pilot plant is used to bridge the gap between lab and commercial process with series of experiments and data collection, the trial runs in commercial process are still required. These mean an interruption in plant production as well as risk of failures for at least first few trials cannot be avoided. At the end, this critical path could jeopardize the balance of speed to launch new products and resource spent significantly.

Considering the computerization technology, which is exponentially advance nowadays, it potentially enables a number of things in the process simulation area, which never been done before. Therefore, the integral modeling is explored and developed as new approach to accelerate petrochemical product development. The architecture of integral modeling consolidates model elements among process simulation, customized modeling, and Computational-Fluid-Dynamics (CFD). The integral modeling aspect takes very high precision of kinetics and hydrodynamics information into account by using and linking multiple software platforms together. This approach improves model prediction far-better than conventional approach which considers either kinetics reactions or mixing phenomena independently.

The advantage of integral modeling could reduce the gap of scaling-up by foreseeing process phenomena in 'virtual' commercial plant with new operating conditions needed for new products. A case study is illustrated with polyethylene (PE) production modeling concept in comparison between conventional and integral modeling technique. With capability of the integral modeling, it can expedite not only launching new products to markets but also speeding up technology development right from proof-of-concept stage through commercialization by reducing plant trials, production losses, and operational risks.

[1156]

NSF Programs and Initiatives in Process Systems Engineering

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The US National Science Foundation (NSF) is an independent agency that funds research in all disciplines at approximately 2,000 universities in the US. Manufacturing research is presently a focus area and being supported by the Obama administration in numerous agencies including NSF. Recent workshops in Process Intensification and Smart Manufacturing as well as previous reports on the research gaps that exist in this area, are leading to new programs and initiatives throughout the Foundation. These are focused on innovation, big data, cybermanufacturing, etc., and are beginning to incorporate other high priority areas such as the food/energy/water nexus, and sustainability.

Track 0. PSE-CAPE and Education

[385]

Experiences in using Operator and 3D Immersive Training Simulators in the Undergraduate Chemical Engineering Curriculum

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In this paper, the authors will discuss their collective experiences in using an operator trainingsimulator (OTS) and an immersive training simulator (ITS) to educateundergraduate chemical engineering students. An OTS is a high-fidelity dynamic model of a chemical process with afront-end human machine interface (HMI) that emulates the plant operation andcontrol room feel of an operating chemical process. Such systems are routinely developed and used in the chemical, power, and nuclear industries to train plant operators (and engineers) on how to operate the process of interest. Plant operations such as cold start-up, shut-down, and normal operations may be simulated. The OTS can also be used to test the skill and ability of an engineer or operator to respond and control unforeseen/abnormal situations through the use of programmed malfunctions. In conjunction with the OTS, a 3D ITS system is also available at the AVESTAR (Advanced Virtual Energy Simulation Training And Research) Center at West Virginia University. The dynamic simulator and its human machineinterfaces (HMIs) are based on the DYNSIM and InTouch software, respectively, from Schneider Electric. The ITS provides an accurate, realistic 3D rendering of the complete plant through which an engineer oroperator may move an avatar in order to observe equipment from the outside as well as inside, observe trends of important variables, open and close valves, and start and stop motors. The operation of the equipment in the ITS is linked to the OTS such that the simulation of field operations are accurately reflected in the dynamic simulation and displayed on the HMI. At present, the OTS and ITS have been used in several courses: a new process simulation course, the traditional process control and the process design courses. In the process simulation course, concepts of steady-state and dynamic simulations as well as digital logic and equipment permissive states were covered. Students were briefed about start-up procedures and the importance of following a predetermined sequence of actions in order to start-up the plant successfully. Student experience with the dynamic simulator consisted of a six-hour training session in which the Claus sulfur capture unit of the IGCC plant was started up. The concepts learned during the training sessions were further reinforced when students developed their own DYNSIM models for a chemical process and wrote a detailed start-up procedure. In the process design course, a module was organized in which the students were introduced to basic principles of equipment layout and placement. Through the enhanced features of the ITS, students were able to "look"inside equipment and see how it operated. Examples of cavitation in pumps and high and low alarms for different equipment were demonstrated. In the process control course, students learned about the dynamic response of a process to changes in manipulated inputs and disturbances and how the control system impacts plant performance, stability, robustness and disturbance rejection. The OTS provided many examples of the complexity of "real-life" process plants consisting of hundreds of pieces of equipment. Students implemented ideal forcing functions, tracked the time-delay through the entire plant, studied the response of open-loop unstable systems, and learned "good practices" in control system design by taking in to account the real-world events where significant deviations from the "ideal" or "expected" response can occur. The overall success of using the OTS and ITS in these courses along with student feedback will be discussed.

[392]

Process Simulators: What Students Forget When Using Them, Their Limitations, and When not to Use Them

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Process simulators allow students to perform in-depth analyses of chemical process designs, including economic optimization, due to the ability to run multiple case studies rapidly. However, process simulators are not necessarily a panacea. Students often use them carelessly. Process simulators have their limitations in dealing with certain types of problems, like debottlenecking and troubleshooting. If it is assumed that most undergraduate students are not prepared to write what Aspen Plus calls "calculator blocks," there are times when a simulator cannot be used.

One example of careless use of a process simulator is when a zoned analysis is needed for a heat exchanger. Many chemical processes have a liquid feed that must be vaporized and superheated before entering a reactor. Heat curves (temperature vs. length or heat transferred) can be plotted in all simulators; however, our experience is that students usually forget to look at them. The typical interface for a heat exchanger in a simulator requires one input for a heat transfer coefficient, which does not correctly model a multi-zone heat exchanger. Each zone must be treated as a separate heat exchanger. Another example occurs when students are taught about heat integration and include it in a design. A heat exchanger that, for example, uses a reactor effluent stream to help preheat the reactor feed might have a close temperature approach. It is very common to see a 1-2 exchanger used without regard for the low, or even impossible, log-mean-temperature-difference correction factor. Another commonly observed situation is a reactor with heat exchange that is way oversized, because the concentration profiles were not examined, and the product composition has either leveled out or begun to decrease due to side reactions. Experience shows that it is one thing for students to answer questions about selectivity in a reaction engineering class, but it is different when they have to recognize poor selectivity in the context of a simulation.

Performance problems such as scale-up, debottlenecking, or troubleshooting are also not always handled well with process simulators. For example, when scaling up a heat exchanger, the heat transfer coefficients change with the flowrate, so this must be included in the analysis. A correct analysis requires including the proportionality between individual heat transfer coefficient and flowrate (to the 0.8 power in turbulent flow, for example), which is not possible in the standard simulator environment. Similarly, reactor cooling loops must include this heat transfer analysis along with the pump performance curve.

When distillation columns are simulated, the heat load on the condenser and reboiler are calculated, but the heat exchangers are not designed. Therefore, when trying to simulate performance of existing equipment under different conditions, the simulation should be modified to remove the heat exchangers from the distillation column and simulate them separately with fixed areas and changing heat transfer coefficients. There is also other peripheral equipment in a distillation column, such as a reflux drum and a reflux pump, which are not simulated in the typical simulator model.

Examples of these and other similar situations will be presented, along with suggested methods for teaching students to simulate their processes correctly. It is hoped that the audience will participate and suggest other examples of the limitations and careless use of process simulators.

[573]

Learning to solve mass balance problems through a web-based simulation environment

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Being able to solve mass and energy balance problems on any given process is a key skill required by students in chemical, or, in general, process engineering. Yet, many students have serious problems solving such problems even in their simplest form, probably because there are no standard equations to use; the balance equations follow the general preservation principles but they must be tailored to the problem at hand.

To solve mass and energy balance problems, students must first identify the system(s) around which preservation equations can be written, the chemical components present and, from all possible balance equations, choose those that, based on the available data, will lead faster to results. In a typical process simulator, there is considerable predefined structure in the form of the data entered and the degrees of freedom are a priori respected during the data entering process. In a typical textbook problem, this is not the case; obviously, in a well-posed problem, the degrees of freedom are respected but there is no predefined structure in the input data (for example, a stream may be only partially known with information on some components missing). So, a process simulator is not the right environment to teach mass and energy balances.

We have developed a web-based environment that imitates the mental process of solving mass balances by identifying in a stepwise fashion the smallest subset of equations which, based on the available data, can more easily yield results. A student does not use degrees of freedom analysis on the entire set of data nor can he/she solve large sets of equations with many unknowns; the web environment respects those restrictions.

The webpage embodying this problem solving environment is formulated around a single continuous process with a collection of options on its input/output structure. The user first selects the input/output structure, declares the chemical components present and then enters the available data on the streams. The provided data fields represent the total flow of a stream and its composition with respect to component mass fractions and component flows. As data are entered, an algorithm checks whether any of the unknown variables can be calculated by applying mass balance equations in any possible combination or by applying constraining equations on the stream itself (e.g., the sum of all mass fractions should be 1). Variables that potentially can be calculated are blocked from data entering and highlighted on the page. Users should, at that point, wonder why these variables are blocked and what equations can be used to calculate them. If they cannot find the answer by themselves, a pop-up message, activated when the mouse hovers above the corresponding fields, shows what equations to use. This procedure continues until all variables on the problem become known.

A separate webpage implements the same environment for batch processes. Through these webpages, users can solve their own problems or practice on predefined problems displayed at the bottom of the page in the form of multi-choice quizzes. The expectation is that such an environment of free, student-centered experimentation can provide structure and guidance on the mental process of how to formulate and solve mass balance problems.

[855]

Model Predictive Control of Post-Combustion CO2 Capture Process integrated with a gas-fired power plant

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The process of CO2 capture and storage is a promising and effective way to control the emissions of CO2 from large-scale power plants. One of the most used CCS strategies is the post-combustion CO2 capture process using MEA. However, the a gas-fired power plant has to respond to dispatching signals from the transmission operator in order to provide load balancing, but frequent changes in operating point create significant disturbances to the CO2 capture plant. Therefore, the integration of CO2 capture process and power plants will increase the need to design advanced model-based control systems to overcome the process interactions and maintain dynamic operability of power plant and CCS unit. Almost all the control schemes that have been recently proposed for the CO2 capture process are focused on decentralized multi-loop control schemes [1-4].

In this work an advanced MPC control scheme has been designed to evaluate the controllability of a post-combustion plant in the presence of disturbances, originated from the different operational schemes from the power plant. Based on the approach developed in [5] an optimisation problem has been developed which gives the set-points for the controllers. The CO2 process was considered as two sub-systems. The first includes the absorber and the second one the stripper.

The liquid MEA-based, post-combustion CO2 capture system was simulated in Aspen Dynamics, while the MPC-based control scheme was implemented using Matlab and the Model Predictive Control Toolbox. Based on data exported by the Aspen Dynamic models the identification toolbox in Matlab was used to obtain the models for the two systems; one SISO and one MIMO system and two MPC controllers have been developed. The performance of the proposed MPC strategy for the CO2 capture plant was validated by applying it on the non-linear process model by a connection established between Matlab and Aspen Dynamics.

In order to validate the proposed control strategy two scenarios have been considered: i) minimisation of steam used in the reboiler with a CO2 capture constraint, ii) minimisation of the CO2 emissions within the steam reboiler constraint. The results have shown that the implementation of the MPC formulation proves to be the best option to address such complex problems in CO2 capture.

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[919]

A Framework to Structure Operational Documents for Chemical Processes

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In the chemical process industry, it is well accepted that operational documents such as operating procedures and manuals are often inadequate and ineffective. As a result, it is widely recognized that these inadequate and ineffective operational documents contribute substantially to the occurrence of plant downtime and often costly and dangerous industrial incidents.

The key reasons for these poor documents are that the original operational requirements from plant owners are not clear, and the fundamental design intentions and design rationales by process designers are not incorporated into these operational documents. This is because the operational design for chemical processes is performed by the process designers during the process design phase, and, in a largely separate exercise, operational documents are created by the plant owners. This decoupling of design and operations means that these documents don't cover all the necessary operation modes and they don't support the design intentions and design rationales.

This paper presents a logical methodology and data structure whereby the key operational design information is carried through into operational documents producing efficient, easily understood and flexible procedural documents that will ultimately result in safe and efficient operations.

To achieve this, first, we identify the clear operational requirements of the plant owners by utilizing the systematized business process model for plant lifecycle engineering that we have developed. Next, we clearly define the business processes of operational design to identify essential and valuable information for plant operation. In particular, with regard to the description of equipment and procedures, we apply the design philosophy of ANSI/ISA-88 to the methodology. (ANSI/ISA-88 is a widely accepted industry standard addressing batch process control). Finally, we integrate these techniques to construct effective, structured operational documents. Documents structured using this methodology reflect all the underlying design intentions/rationales and operation modes and, at the same time are easier to use and easier to maintain. We propose that this will substantially contribute to safer and more efficient operations in industrial sites.

[1146]

Teaching Sustainable Process Design Using 12 Systematic Computer-Aided Tasks

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In this paper a task-based approach for teaching (sustainable) process design to students pursuing a degree in chemical and biochemical engineering is presented. In tasks 1-3 the student makes design decisions for product and process selection followed by simple and rigorous model simulations (tasks 4-7) and then sizing, costing and economic analysis of the designed process (tasks 8-9). This produces a base case design. In tasks 10-12, the student explores opportunities for heat and/or mass integration, followed by a sustainability analysis, in order to evaluate the base case design and set targets for further improvement. Finally, a process optimization problem is formulated and solved to obtain the more sustainable process design. The 12 tasks are explained in terms of input and output of each task and examples of application of this approach in an MSc-level course are reported.

Track 1. Modelling, Numerical Analysis and Simulation

[10]

Uncertainty in Clinical Data and Stochastic Model for In-vitro Fertilization

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In-vitro Fertilization (IVF) is the most common technique in Assisted Reproductive Technology (ART). It has been divided into four stages; (i) superovulation, (ii) egg retrieval, (iii) insemination/fertilization and (iv) embryo transfer. The first stage of superovulation is a drug induced method to enable multiple ovulation, i.e., multiple follicle growth to oocytes or matured follicles in a single menstrual cycle. IVF being a medical procedure that aims at manipulating the biological functions in the human body is subjected to inherent sources of uncertainty and variability. Also, the interplay of the hormones with the natural functioning of the ovaries to stimulate multiple ovulation as against a single ovulation in a normal menstrual cycle makes the procedure dependent on several factors like the patient's condition in terms of cause of infertility, actual ovarian function, responsiveness to the medication. The treatment requires continuous monitoring and testing and this can give rise to errors in observations and reports. These uncertainties can be observed in the form of measurement noise in the available data. Thus, it becomes essential to look at the process noise and think of a way to account for it and build better representative models for follicle growth. The purpose of this work is to come up with a robust model which can project the superovulation cycle outcome based on the hormonal doses and patient response and hence provide a treatment guideline to enhance the success rate of the procedure.

[34]

Thermally Coupled Distillation Sequences for the Separation of Quaternary Mixtures: Effect of the Feed Composition on Energy Consumption

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Distillation is among the most used unit operations for the separation of fluid mixtures. It takes advantage on the differences on boiling points of the components of the mixtures. Nevertheless, this operation has an inherent low second—law efficiency, then it has high energy requirements and, as a consequence, high environmental impact. In order to reduce energy requirements for the distillation units, alternative configurations have been proposed. Such configurations are known as thermally coupled distillation sequences, and it has been shown that it can reduce considerably the required heat duty, in comparison with conventional sequences. Nevertheless, the reduction on energy requirements depends considerably on the feed composition and the nature of the mixture. Tedder and Rudd presented a map of the compositions for which thermally coupled systems for ternary mixtures allowed low energy requirements. Nevertheless, to the knowledge of the authors there is no information about the compositions for which quaternary thermally coupled systems show lower energy requirements than conventional sequences. Thus, in this work, an analysis of the impact of feed composition on the energy requirements of thermally coupled distillation sequences for quaternary mixtures is presented. The set of compositions to be analyzed is obtained through an experimental design approach. The design and optimization of the distillation sequences is performed through a multiobjective genetic algorithm with constrains handling.

[55]

A framework for a direct exploitation of available information in the online model-based redesign of experiments

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MBDoE aims at designing a set of experiments yielding the most informative process data to be used for the parameter estimation of first-principles dynamic process models. According to the standard procedure described in literature [1], the experiment is generally designed offline; then it is carried out in the plant/lab, process measures are collected and parameter estimation is carried out only at the end of the experimental run: since the experiment is designed on the basis of the initial available parameter estimates, the progressive increase of the information resulting from the progress of the test is not exploited. In order to overcome this problem new techniques were proposed [2,3], where the information is exploited as soon as it is generated by the execution of an experiment by redesigning the experiment online through intermediate parameter estimations. This technique enables users to reduce the number of experimental trials needed to reach a statistically sound estimation of model parameters and results in a substantial reduction of time and costs. Nevertheless, this technique exhibits some limitations potentially hindering the effectiveness of the redesign procedure: on the one side, the time point at which redesigning the experiment is chosen "a-priori", without verifying whether enough information has indeed been collected to obtain an improvement in the estimation of the parameter value; on the other hand, the first design may be heavily affected by the initial parametric mismatch.

In order to overcome those problems a new strategy is here proposed. The main advantages is that a robust approach [4] is adopted within the online redesign procedure and, most importantly, a new design criterion based on the maximisation of a target profile of dynamic information is introduced. The methodology allows determining when to redesign the experiment in an automatic way, thus guaranteeing that a sufficient increase in the information content has been achieved before proceeding with the intermediate estimation of the parameters and the design of the experiment. Furthermore, the robust approach allows reducing the negative effects of the initial parametric mismatch. The effectiveness of the new experiment design techniques is demonstrated through a simulated case study.

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Optimization of Chemical Processes Using Surrogate Models based on a Kriging Interpolation

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In this work, we present a methodology for the rigorous optimization of chemical processes implemented on a commercial simulator using surrogate models. Sometimes, in nonlinear programming problems, the objective function and/or some constraints of the problem are given by implicit grey box functions that introduce noise. The aim of this work consists of replacing some of these functions by surrogate models based on Kriging interpolation [1,2]. Kriging is an interpolation method whose functions contain adjustable parameters. The quality of the model depends on the number of independent variables and the narrowness of their bounds. Surrogate models can be used following different approaches. We can replace a complete model (i.e. complete flowsheet). We can also substitute one or some of the components of the model (i.e. unit operations). Or finally, we can develop a local approach of the complete model or some of its components. In this work, we use a combination of models. On the one hand, some units operations that need a notable CPU time and also introduce noise (reactors and distillation columns) are replaced by Kriging metamodels. On the other hand, the rest of the flowsheet (as mixers, splitters…) are represented by an accurate model.

To calibrate the surrogate model of the selected unit operations, we have to establish the lower and upper bounds of the independent variables. We generate sampling points distributed around the search area using a min-max approach (minimizing the maximum distance between two points). We simulate the unit operation with Aspen HYSYS v.7.3 in each sampling point. Finally, we use the values of the variables of each simulation to calibrate the Kriging parameters. We can optimize a problem quickly replacing unit operations by their surrogate model.

If the metamodel is used as an implicit model in which each iteration corresponds to an external equation, we can ensure just a local optimum. On the other hand, it is possible to obtain a global optimum if the surrogate model is used as a set of explicit equations included in the MINLP optimizer. In the first case, the solver deals with a robust and small model. In the second case, the solver finds a larger model that is limited to a small number of metamodels.

Several examples were studied. We performed the optimization of different conventional distillation columns, sequences of columns, an extractive distillation system and some superstructures. Thus we noted the efficiency and effectiveness of the method. It is also planned performing more complex superstructures that include both reactors and distillation columns.

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Global Sensitivity Analysis for a Dynamic Model of Chronic Lymphocytic Leukemia Disease Trajectories

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In the United Kingdom, B-cell Chronic Lymphocytic Leukemia (CLL) is the most common form of leukemia with 2,800 people diagnosed annually; 75% of these patients are older than 60 years of age. Unlike acute leukemias, which typically involve uncontrolled growth of immature blood cells, CLL is usually a slowly progressive malignancy of mature B-cells arrested in the cell cycle phase G0/1. CLL couples abnormal growth with resistance to apoptosis (programmed cell death).

There is an unmet need to mathematically simulate the dynamic disease trajectory of cancers, such as CLL, in the human body; these models may improve clinical pathways for cancer treatment and enable personalized healthcare. Using a prior mathematical model of acute myeloid leukemia as a springboard, we have developed the first dynamic, physiologically-relevant mathematical model of CLL interconnecting affected tissues in the relevant disease centres: peripheral blood, lymph nodes, spleen and bone marrow. Our CLL model captures patient heterogeneity across disease states including monoclonal B lymphocytosis (a CLL precursor) and more aggressive disease stages. This manuscript analyses our CLL model with respect to prior work that applying global sensitivity analysis to nonlinear dynamic models of biological systems. We exploit the high dimensional model representation (HDMR) method for global sensitivity analysis that finds input-output relationships of a complex model with a high dimensional input space. The high dimensional input space consists of: (1) apoptotic rates of cancerous cells in each affected tissue evaluated from in vivo and in vitro studies; (2) migration rates of cancerous cells; (3) time spent in the cellular proliferation phase; (4) rate of recruitment cells from the non-proliferative phase to proliferative phase. Model outputs are the numbers of cancerous cells both in proliferative and non-proliferative cell cycle phase of each affected tissue.

This manuscript shows how global sensitivity analysis of our physiologically-relevant model reveals what may be key clinical parameters for patient treatment. We show how the critical model parameters relate to measureable patient data for capturing heterogeneous leukemia dynamics; this personalized model suggests personalized treatment of CLL disease progression. This effort belongs to the Biological Systems Engineering Laboratory and the Centre for Process Systems Engineering at Imperial College where we develop building blocks of a design framework for modeling and optimization of biomedical systems.

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Optimization of LNG Plant Operating Conditions to Anticipate Leaner Feed Gas by Steady State Process Simulation

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Badak LNG has operated for producing LNG more than 36 years, with total production capability of 22.5 million metric ton LNG per annum. Badak LNG has eight (8) LNG Trains which was designed with specific range of feed gas composition. In the future, regarding with developing of new gas wells, it is predicted that new gas wells have leaner gas composition than current feed gas. Thus, it could impact to performance of LNG plant especially in refrigeration and liquefaction system. An evaluation is required to find out the potential restrictions and new operating condition when liquefying the leaner gas. By using simulation model of LNG plant, the effect of lean feed gas basically could be predicted. The simulation is firstly validated by using the actual performance data. Afterwards, it is used to simulate the leaner gas with optimization methods. The optimal model simulation uses specific energy as objective function, the refrigerant flow rate and composition as operating variables while the existing equipment's capacity is used as parameter constraints.

The evaluation result concludes that liquefying the leaner gas will need more refrigerant flow rate to keep minimum temperature approach at Main Heat Exchanger, so the power and specific energy also increases while LNG product flow rate decreases. The inlet temperature of refrigerant compresor is potentially colder than minimum speification of -45 degree C, it will be a constraint when processing the leaner gas. But, optimizing the operating condition such as flow rate, pressure and composition of refrigerant, can reduce compressor power and specific energy while temperature inlet compressor still meet the specification.

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Modelling and Simulation of Complex Nonlinear Dynamic Processes Using Data Based Models: Application to Photo-Fenton Process

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Accurate mathematical First Principle Models (FPM) are essential for the understanding of chemical processes. However, complex processes usually lead to complex mathematical models (i.e. highly nonlinear, including implicit parametric functions, and/or ill formulated). Even when these models are available, practical challenges may appear when using them, so requiring high computational time and effort for their solution. In these situations, surrogate modeling or system identification techniques provide an efficient alternative option to construct simplified predictive dynamic models using input/output simulation or real data or both.

This paper investigates data based modelling of complex nonlinear processes, for which a first principle model useful for process monitoring and control is not available. These empirical models may be used as soft sensors in order to monitor a reaction's progress, so reducing expensive offline sampling and analysis. Three different data modelling techniques are used, namely Ordinary Kriging, Artificial Neural Networks and Support Vector Regression. A simple case is first used to illustrate the problem, assess and validate the modelling approach, and compare the modelling techniques. Next, the methodology is applied to a photo–Fenton pilot plant to model and predict the reaction progress.

The results show how data based models can be used as soft sensors to monitor complex processes, difficult to follow through FPMs, without expensive offline sampling, saving huge costs and time. In addition, a simple static modelling approach has shown to be capable of accurately estimating a dynamic behaviour. Based on the proposed approach, the three data modelling techniques have been built to infer the progress of a chemical process from cheap on-line data. The results produced reveal that all methods exhibit high prediction accuracy with a significant low number of training data. Especially, Kriging shows a slightly higher accuracy and more importantly, higher flexibility and robustness in terms of easiness and rapidness of tuning the model parameters, while providing the modeller with a quantitative confidence interval of the prediction.

Acknowledgements

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A Meshfree Maximum Entropy Method for the Solution of the Population Balance Equation

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The population balance equation (PBE) is a transport equation with integral and nonlinear source term. The analytical solutions of this equation are generally of academic interest and are available only for a few cases with restricted interaction kernels. In this contribution, we propose a novel meshfree converging sequence of continuous approximations to the number concentration function as a solution to the PBE using the Maximum Entropy (MaxEnt) principle, where particle growth and breakage are included. The solution appears as the Shannon MaxEnt functional, which is forced to satisfy the regulatory conditions imposed by the number concentration function for the particle size distribution. The natural logarithm of the MaxEnt functional is expanded using a complete set of orthogonal basis functions, which satisfy the regularity conditions. The coefficients of the expansion are estimated using local information about the number concentration function, which is carried by the field nodes.

As a case study, the method is applied to solve the microbial cell population balance dynamics which includes cell growth and division in a constant abiotic environment. Additional assumptions are placed on the growth and division rates and daughter cell distribution function to get a dynamic analytical solution. The Adomian method is used to obtain this analytical solution [1] which is compared to the meshfree MaxEnt method. The dynamic evolution of the microbial cell population in a chemostat with zero dilution rate and a constant substrate concentration has been obtained. The intercellular state is represented by the cell biomass which reflects its size (length). The meshfree MaxEnt method captures with a high accuracy the evolution of the population dynamics using only 10 field nodes. Note that, due to simultaneous cell growth and division the cell density evolution to the small size range is slower when only cell division is dominant.

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Modelling the Hydrodynamics of Bubble Columns using Coupled OPOSPM-Maximum Entropy Method

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Bubble columns are multiphase equipment which is widely used in the chemical, petrochemical and biochemical industries. The gas phase is dispersed in a continuous environment with a population of bubbles that may undergo breakage, coalescence and growth. Modelling such a process using the mixture models, which fail to take into account these instantaneous discrete events, is not sufficiently accurate to predict the hydrodynamics and mass transport in such equipment. In this contribution, we used a reduced population balance model to describe such events, which play a major role in in determining the bubble size distribution and hence the interfacial area concentration. The reduced population balance model consists of a set of transport equations to track the total number concentration, total interfacial area concentration and gas phase volume fraction of bubbles. This model is essentially derived using the One Primary and One Secondary Particle Method (OPOSPM), which is coupled with the Shannon Maximum Entropy Method (MaxEntM) to predict the bubble size distribution along the bubble column axial direction.

The first results show that the present model can be extended to higher-order approximations of the population balance equation using more secondary particles. This is an obvious advantage over the existing models such as that of Hibiki and Ishii [1]. As a first step of model validation, the pilot plant bubble column of Hibiki and Ishii [1] was modeled and simulated after the necessary modifications of the breakage and coalescence kernels to recover the mathematical consistency with the population balance equation. The variation of the gas holdup along column height (~ 3m height) and the recovered bubble size distribution has been compared to the experimental data [1]. As discussed by Hibiki and Ishii [1], the simulated bubbly flow is dominated by bubble expansion due to the axial pressure drop along the column height, which is reflected by the mean size of the MaxEnt bubble size distribution.

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Process Simulation of a 420MW Gas-fired Power Plant using Aspen Plus

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Carbon Capture and Storage (CCS) is known as a promising route for controlling the global warming [1]. Amine scrubbing is probably the only technology for Post-Combustion Capture (PCC) for CO2 that is available to those existing power plants [2]. The challenges on the way in implementing the process for treating the entire flue gas of a full size power plant is how to obviously reduce the exceeding high energy requirement for solvent regeneration [3] and how to integrate the PCC with those existing power plants.

It is believed that combustion of natural gas is the most efficient means for generating electricity from fossil fuels[4]. However, only one paper thus far is found to simulate the gas-fired power plant, and just general and some key data rather than detailed information was reported4. Obviously, such information is far from enough to lay a basis to carry out an effective integration of PCC to a gas-fired power plant. Under such situation, a typical 420MW gas-fired Combined Cycle Power Plant (CCPP) in Europe is modelled and analysed in detail. It consists of four sections: (1) natural gas preparation, (2) gas turbine, (3) Heat Recovery Steam Generation (HRSG) and steam turbine, (4) water recycle system. The model was developed using Aspen Plus software of version 8.0[5]. Comparing with the operating data of the commercial plant, the simulation results are in good agreement with the operation data.

The novelties of this paper are: (1) the most complete process model of a gas-fired CCPP thus far is built and validated by operating data. The boundary of the model covers the whole range of the CCPP; (2) much more detailed and rigorous models of gas turbine and HRSG than ever before are built although some key parameters cannot be disclosed to protect the power plant; (3) potential integration options with PCC are proposed and analysed.

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Optimal blending study for the commercial gasoline

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This paper discusses the issue of the commercial gasoline blending. The gasoline thus obtained must be according to the EN 228 and EURO standards. The linear optimization problem is made from the objective function and the restrictions system. The objective function has a financial nature and the restrictions system has mathematical expressions which cover three aspects: a) the quality of the finished product, estimated by a components blending mathematical model; b) components quantities; c) variables non-negativity restrictions.

For a flexible solving of this problem, the authors have elaborated a dedicated software starting from the Simplex algorithm proposed by Jean-Pierre Moreau. The input data of this program are structured in four categories: the utilized components and its properties; available quantity and components process; the properties used as restrictions and the total amount of commercial gasoline that must be obtained. A big part of the input data can be selected by the user from a predefined list.

Using the optimization program were studied the optimum blending recipes from the following variants: 1) Recipes that take into account a single restrictive property; 2) Recipes that take into account two restrictive properties; 3) Recipes that take into account a single restrictive property but have a default bioethanol proportion in the final blending.

For the first variant, the dependence between was the restrictive property's value of the optimum blending recipe with the total blend quantity and the variation of the component quantity with the total blend quantity. For the second study variant were analyzed all the possible combinations of two properties from the nine possible properties, 28 variants being studied in total. The obtained results in these two variants allowed the study of the blending properties variance with the utilized components quantity.

The third study variant followed the solving of a real problem in the commercial gasoline blending process, obtaining a commercial gasoline with an imposed bioethanol content. Variants which have between 1 and 5% vol. of bioethanol were analyzed, for each variant being followed the commercial gasoline properties.

The obtained results validated the software tool and the analysis methodology of the optimum blending recipes for obtaining commercial gasoline.

[139]

Population balance model for enzymatic depolymerization of branched starch

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Starch is a large (mean amount of monomer units up to 106) and highly branched (average of 1 branching per 20 bonds) biopolymer with a broad distribution in amount of monomer units. Because many plants produce it to store energy, it is one of the most abundant polymers in the world. In several industrial processes (e.g. the mashing process) starch is depolymerized into saccharides by enzymes. The saccharides might be used as the feedstock for a fermentation process. The performance and economic feasibility can be improved by using an optimal temperature profile or an optimal enzyme concentration.

In order to perform optimization without having to run many experiments accurate simulation techniques are desired. Like most bioproducts starch has a large variability which might necessitate performing the optimization for each specific batch run. Eventually, even a real-time control is desirable. Then, efficiency of the simulation techniques becomes crucial. The first models proposed to describe the depolymerization of starch used a very simple reaction scheme that is unable to reproduce experimental results. Recent models were solved using Monte Carlo techniques. This enables consideration of the full complexity of reaction and substrate. However, Monte Carlo techniques are computational very expensive. A more promising approach is to develop and use a population balance model.

In this work such a model is developed for one of the important enzymes (α-amylase). One problem in using a population balance for polymers is the unavailability of the polymer structure which hinders the inclusion of sterical effects. The authors propose a novel method to overcome this limitation. A model for the reaction rate that has proven to be suitable to describe the depolymerization of linear starch is employed and adapted for branched polymers. The population balance model is solved using a novel numerical algorithm recently developed by the authors.

A preliminary comparison of the simulation results to experimental data is undertaken in this work. The qualitative nature of the measured data is reproduced. Reasons for the deviations are discussed and improvements to the model are suggested.

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Analysis of the transfer of radical copolymerization systems from semi-batch to continuous plants

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The production of copolymers with different reaction rates of the two monomers is nowadays mostly done in discontinuous batch or semi-batch plants. The idea of transferring the advantage of product flexibility to the continuous mode of operation has been investigated during the European research project F3 Fast Flexible Future Factory [1]. The continuous plants considered for co-polymerizations of monomers with different reactivities are modular plug-flow reactors (PFR) with side injections. By the switch to continuous production, the continuous feed of reactants is replaced by lumped feeds at the injection points. This poses the question for which copolymers it is possible to obtain the same product in the continuous mode of operation as in the semi-batch mode. If this is possible, the better heat transfer characteristic in the continuous plant enables higher production rates and space-time yields which together with the improved uniformity of the production makes continuous production an interesting alternative. As the transfer of a batch process to a continuous PFR plant is restricted by the minimum flow velocity for sufficient heat transfer and the possible residence time in the PFR, the transfer of a semi-batch process to continuous mode is non-trivial because the addition of feeds to the process is, in contrast to the semi-batch process, limited in range and space.

During this work the possible product range of copolymers that can be transferred from semi-batch to continuous mode is determined by a screening method. This method is based on the description of the polymerization reaction of two different monomers by six kinetic parameters. The kinetics of the copolymerization is described by a reduced terminal model. The parameters are two reactivity ratios, and the ratios of homo-propagation rates and termination rates. Applying constraints on both processes like minimum conversions of the monomers and the cooling capacity, feasible processes are determined by the variation of the feed rates. The range of product qualities can be analysed in the space which is spanned by the input parameters. Within the range of the product qualities the most important qualities can be detected and used as criteria for the transfer from semi-batch to continuous production. The knowledge of the feasibility limits for both processes provides overlapping regions, for which a direct transfer without significant changes in product quality is possible and information on the differences in the product qualities of the two modes due to the transfer to the continuous plant. For reaction systems for which a direct transfer is possible, an optimization within the overlapping region of product qualities can be performed to compute the maximum throughput of the continuous plant and thus the maximum increase of the space time yield compared to the discontinuous plant.

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Thermodynamic Considerations for Systems Biocatalysis

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'Systems Biocatalysis' is a new concept for constructing multi-enzyme processes in vitro for the synthesis of chemical products [1]. This artificial metabolism is controlled in an efficient way in order to achieve a sufficiently favourable conversion for the target product. However, many biocatalytic processes are unfavourable and often limited by thermodynamics where the equilibrium position of reaction lies to the reactants rather than the products. For instance, w-Transaminase (EC.2.6.1.X) reaction theoretically can produce a 100% yield of chiral amine (a building block for pharmaceutical products) from ketone. Because of thermodynamic limitations, a lower product concentration is frequently achieved [2]. Such thermodynamic-challenged reaction can be improved by changing the thermodynamic environment of the reaction (e.g. temperature and pH) or by coupling with the energetically favourable reactions (energy-releasing reactions such as, alanine dehydrogenase-catalysed reaction, EC1.4.1.1) and/or by coupling with a high energy substrate such as, molecular oxygen, as the driving force to shift the equilibrium position. Such thermodynamic evaluation is fundamentally important in order to apply the concept of the system biocatalysis successfully. Thus, the aim of this work is to estimate the equilibrium thermodynamic properties of biocatalytic reactions using the property prediction tools available such as the group contribution method [3,4] and ab initio quantum mechanics method [5]. The estimated values are useful to predict the feasibility of the process operating strategies and to set realistic targets for the development of such cascades.

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DAE Tools: Equation-Based Object-Oriented Process Modelling, Simulation and Optimization Software

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In this work DAE Tools modelling simulation and optimization software, its programming paradigms and main features were presented. The current approaches to mathematical modelling such as modelling languages and general-purpose programming languages were analyzed. The common set of capabilities required by typical simulation software was discussed and the shortcomings of the current approaches recognized. A new hybrid approach was introduced and the modelling languages and the hybrid approach were compared in terms of grammar, compiler, parser and interpreter requirements, maintainability and portability, needs for runtime model generation and simulation setup, availability of runtime operating procedures, interoperability with the third party software packages, model exchange and co-simulation capabilities. The benefits of an equation-based approach to process modelling implemented in a fourth generation object-oriented general purpose programming language such as Python were discussed. The architecture and the software implementation details as well as the type of problems that can be solved using DAE Tools software were presented. Finally, some applications of the software at different levels of abstraction were presented and its embedding capabilities and suitability for use as a software as a service demonstrated.

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Parallel Computation Method on GPU Platform for Solving Equation-oriented Models

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Equation-oriented approach (EO) is an important method for process simulation and optimization. A large-scale EO model consists of a very large number of nonlinear equations, resulting in the solving process a challenging and time-consuming task. During the solving process, function evaluation of residual errors at each iterates is an essential step. With the EO feature, this step can be parallelized in a natural way. In this project, a parallel computation method on the graphics-processing-unit (GPU) is presented. The function evaluation step is computed in a parallel mode to accelerate model solving. The functions in an EO model are divided into several groups, among which the function evaluations are calculated simultaneously. The implementation of the proposed method on the NVIDIA GPU platform is described. A number of numerical examples are presented to demonstrate the applicability and efficiency. A theoretical analysis on the speedup ratio is also discussed.

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Dynamic investment appraisal: Economic analysis of mobile production concepts in the process industry with agent-based simulation

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Due to technological developments new small scale mobile production concepts have become available in the processing industry. These novel production concepts have mobility as an attribute and the profitability of the production concepts depends, amongst others, on how well this attribute can be exploited as the cash flows of these concepts depend on optimal location choice in volatile markets. The existing cash flow projection methods, used as basis for the investment appraisal, do not take this dynamics into account and are therefore less applicable for projecting the cash flows of these new production concepts. The cash flows emerging from these new attributes are typically disregarded, which may lead to the underestimation of the novel production concepts' value and consequently prohibits their deployment. In this paper we combine an agent-based model simulation with a net present value calculation to appraise these new production concepts. The agent-based model uses a q-learning algorithm to simulate an existing world scale market in which we introduce the new production concepts and let them compete with existing industry. For the new production concepts we measure cash flows from purchased feedstock and sold product that are used in the net present value calculation to appraise the investment. To illustrate the added value of mobility, we apply our approach to a case study in which we appraise a stationary and mobile production concept. We show that simulation can be used to project the cash flows of investments with complex attributes to help improve the quality of investment decisions. In order to be able to quantify other benefits than mobility future work will focus on adding more operational attributes (such as processing duration) of these new production concepts to the model.

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Prediction viscosity of ionic liquid based on COSMO-RS $S_{\sigma\text{-profile}}$

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Ionic liquids (ILs) are considered as an important family of "green" solvent which have attracted much attention for their remarkable properties, such as negligible vapor pressure, thermal and electrochemical stability, non-inflammability and tunable property [1-4].

The viscosity of ionic liquids (ILs) in a chemical engineering process appears to be important in transfer phenomena context as well as practical applications in industry. In addition, to the best of our knowledge, the comparable theoretical basis for the estimation of liquid viscosity has not been elucidated yet [5]. Therefore, it is necessary to predict the viscosity of ILs through various accurate predictive tools.

In this work, two new quantitative structure-property relationship (QSPR) models have been developed for predicting the viscosity of ILs using multiple linear regression (MLR) and support vector machine (SVM) algorithms based on the Sσ-profile descriptors calculated by COSMO-RS. A large data set of 1502 experimental data points of 89 ILs covering a wide range of pressures and temperatures were applied to validate the two models. The experimental and calculated viscosity logarithm values of traing set as well as test set for all ILs have been obtained. The mean squared error (MSE) and the average absolute relative deviation (AARD) of test set of the MLR and SVM are 0.187, 10.61% and 0.025, 6.75%, respectively. The nonlinear model developed by the SVM algorithm is superior to the linear model built by the MLR, which indicates that the SVM algorithm is more reliable in the prediction of viscosity of ILs. Furthermore, the derived models also throw some light on what structural features are connected with the viscosity of ILs.

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[298]

OPOSSIM: A New Population Balance-SIMULINK Module For Modelling Coupled Hydrodynamics and Mass Transfer in Liquid Extraction Equipment

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Dynamic behaviour, control and design strategies for liquid extraction equipment are faced by the complex hydrodynamic behavior of the dispersed phase with many dynamic interactions (e.g. breakage & coalescence). To take this into account, the population balance modelling framework is used by implementing the multivariate OPOSPM (One Primary and One Secondary Particle Method) with a one-dimensional finite volume method in the physical space [1]. In order to provide more realistic information about the equipment dynamic behavior, and to narrow the gap between the steady state and dynamic design during process synthesis, OPOSPM is implemented in a MATLAB/Simulink flowsheeting environment. As an outcome of this, we present a new OPOSPM-MATLAB/Simulink module which is called OPOSSIM for modeling and simulation the coupled two-phase flow and mass transfer in liquid extraction equipment. For general simulation purposes, the PPBLAB data exchange interface is adapted to allow full access to the thermodynamics package (TEA), which is provided by CAPE-OPEN Simulation Environment. Moreover, the MATLAB Graphical User Interface is utilized to design user-friendly windows input dialogs in order to define all the

The performance of OPOSSIM has been tested against steady state and dynamic experimental data at different operating conditions using different chemical test systems (water-acetone-toluene and water-acetone-butyl acetate). A comparison has been performed between the simulated dispersed phase holdup dynamic responses and the experimental data [2] in a Kühni extraction column due to combined step changes (positive and negative) in the total throughput.

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[304]

Modelling of sugar removal by dia-ultrafiltration of commercial food colorant and viscosity influence on permeate flux

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Additives from natural origin are increasing in popularity in the food industry because of the increased consumer focus on a healthier life style based on organic food. In the case of blue colorants, one of the most popular natural sources is the microalgae Spirulina platensis. Some examples of food products in which Spirulina-based colorants are used are cakes, candies, beverages or ice-creams.

The blue color of Spirulina-based colorants is caused by phycobiliproteins, in which the chromophore part, a tetrapyrrole group, is bound to the proteic part of the molecule. In order to preserve the color during shelf life, protein mixtures are commercialized in combination with sugars and citrate salt. However, the natural blue colorants available in the market sometimes show changes of intensity and hue when exposed to different environments. This could be circumvented by isolating and stabilizing the chromophore. Isolation and stabilization of the chromophore can be achieved by chemical alteration, but in order to prevent undesired side reactions a protein mixture free of additives is preferred. The difference in size between the proteins and additives is compatible with a size exclusion separation process such as membrane technology.

In the present work, a mathematical model based on experimental dia-ultrafiltration on colorant solutions using water as diafiltration solvent is developed. Model solutions with different concentrations of sugars and citrate salt have been tested on the same process with the aim of evaluating the effect of viscosity in the permeate flux. Moreover, different concentrations of colorant have been tested to quantify the resistance caused by the protein gel layer formed at the membrane surface. Comparison of diafiltration performance of the model solutions with protein colorant mixtures has made it possible to model the mass transfer across the gel layer and the membrane, and implement a prediction model for the permeate flux decay.

[311]

Effect of cryogenic air separation purity on oxy-fuel combustion for carbon capture

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Oxy-fuel combustion has been widely identified amongst the most promising technologies for carbon capture and for achieving significant reductions in greenhouse gas emissions in a cost effective manner. By replacing air with nearly pure oxygen, the combustion is carried out in conditions that result in a flue gas stream rich in carbon dioxide that can easily be further purified before being sent to compression and sequestration.

In an oxy-fuel combustion system, the downstream purification of the CO2 rich stream is facilitated by the high concentration of CO2, relative to other species in the flue gas, and by the reduced amount of nitrogen oxides, which would form if air were to be used as an oxidant in the combustion. On the other hand, combustion in the presence of a high purity oxygen stream results in a high temperature that needs to be attenuated by recycling part of the flue gas stream. More critically, the cost of producing high purity oxygen on-site, using a cryogenic air separation unit, is the major contributor to the CO2 avoidance costs of oxy-fuel combustion due to its high energy requirements.

The objective of this work is to provide a quantitative measure of the costs and benefits of producing oxygen with different levels of purity, using a cryogenic air separation unit, in the context of a power plant with oxy-fuel combustion, carbon dioxide purification, and CO2 compression. Modelling and simulation is carried out in Aspen Plus.

Initial results on the development of a rate-based dynamic model for cryogenic air separation are also presented.

[316]

CFD-DEM simulation of a fluidized bed crystallization reactor

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CFD-DEM simulations (CFD: Computational Fluid Dynamics; DEM: Discrete Element Method) are multiphase simulations that take into account all interactions occurring between particles and fluid. One speaks of a so-called four-way coupling, which means that 1) the particles can collide with each other and with the reactor walls, 2) the fluid influences the particles, 3) the particles have an influence on the fluid flow. Simulations with many particles require a correspondingly high computational effort, but they can still be carried out using large parallel computers. Due to increasing computational power and to the high physical accuracy of CFD-DEM simulations, this approach is becoming increasingly important for research and industry.

Contrary to solid-gas fluidized beds, CFD-DEM studies pertaining to solid-liquid fluidization are not often found in the scientific literature yet, although this configuration plays an important role in the chemical, pharmaceutical and food industry.

In the present study, an innovative reactor concept developed for the continuous separation of enantiomers is investigated by CFD-DEM simulations. A racemic mixture is separated by selective crystallization in the reactor. For this purpose, the crystals are dissolved in a solution that flows through two parallel fluidized bed reactors. By controlling reactor parameters small starter crystals can be added continuously, and grown crystals (with desired final diameter) are discharged continuously from the fluidized bed. The CFD-DEM simulations deliver important information concerning in particular fluidization limits, bed height, and residence time.

The used software CFDEMcoupling contains a solver that was developed by combining the C++-based open source software environments OpenFOAM (for CFD) and LIGGGHTS (for DEM). The solver carries out the fluid (CFD) and particle (DEM) calculations using two clearly separated codes. This allows to develop and improve both codes independently. The interaction is realized by exchanging relevant fields with a predefined time step. Through parallelization relying on MPI (Message Passing Interface) a good efficiency is obtained on parallel computers.

[321]

A Modelling, Simulation, and Validation Framework for Large-scale Processing Systems with Distributed Management

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Industrial production sites consist of many production plants that are interconnected via networks for materials and energy transfer to enable the re-use and integration of steam, side products, electrical power, etc., and to realize economic advantages of scope. While the operation of the individual plants is managed mostly locally, the optimization of global performance indicators (such as minimal energy and material consumption, or reductions in CO2 emissions) requires a site-wide strategy for demand-supply management. Today, companies mostly rely on infrequent planning of production and consumption and interactive management of deviations in daily meetings or by phone, which leaves a significant potential for optimization due to the existence of many dynamic interactions within a site and with its environment (e.g. changes in production volumes, disturbances, start-ups, shut-downs, product changeovers, short-term variations of the cost of electricity). Automated, optimization-based site-wide management strategies are expected to significantly improve the operational efficiency of large production sites. This coordination has to be performed in a distributed and hierarchical fashion, making use of local automation and optimization and respecting the management structures of the site. Such systems with local decision power and global coordination are termed Systems of Systems. Model-based engineering is indispensable to guide and to validate the design of such large complex management and automation structures and requires the composition of site-wide models from modular descriptions of the different units on different levels of details and complexity.

In this contribution, a new framework is presented that is tailored towards the modelling, simulation, and validation of such large Systems of Systems with decentralized management. The framework, is based on the Modelica language for heterogeneous modelling (see e.g. [1]), and aims at reducing the effort for model creation by providing standard interfaces for the connection of physical process model components of different levels of detail (both existing and newly developed models) as well as management algorithms. The plug-and-play approach facilitates the testing and validation of different management algorithms of an industrial site, and simplifies the integration of new management architectures into an existing system.

The potential of the framework is illustrated on an industrial application example, the model of a significant part of a petrochemical production site.

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[322]

Performance Analysis and Optimization of the Biomass Gasification and Fischer-Tropsch Integrated Process for Green Fuel Productions

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Continuous increase in fuel prices driven by high energy demand and limited fossil fuel resources has been presently considered a major problem for an industrial sector. Moreover, gas emissions from internal combustion engines lead to air pollution and global warming issues. Therefore, the development of clean, alternative energy is required in order to relieve the fossil fuel shortage and environmental impact. A biomass-to-liquid (BTL) process is recognized as a promising technology to convert biomass to liquid fuels. This study focused on theoretical analysis of the BTL process consisting of a gasification unit for synthesis gas production and a Fischer-Tropsch (FT) unit as a downstream process for synthesis gas conversion to liquid fuels. Rice straw, one of the most biomass residuals found in Thailand, is considered as a feedstock. The integrated model of the BTL process consisting of three major sections, i.e., the gasification based on the reaction kinetics of char gasification, the gas conditioning process including tar steam reforming and water gas shift reaction, and the FT synthesis is developed and used to investigate the influence of operating parameters on the product distribution and the overall energy consumption. Two gasification systems using different gasifying agents, i.e., oxygen/steam and air/steam are considered and compared. The optimum conditions that provide the highest yield of a high-valued diesel product with the lowest energy consumption are identified.

[333]

Dynamic behavior adjustment of 1,3-propanediol fermentation process

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Multiple steady-state solutions typically exist for nonlinear chemical processes and the stability of various solutions may be different. Stability is a key component of chemical process operability and represents the tolerance for small perturbations in the process, which is related to process benefits and safety. As one of the multiple steady-state solutions, the optimal operating point may be located in the unstable branch. Even the control system is implemented to form a closed-loop system, stable operations can't be ensured. 1, 3-propanediol is an important chemical material, mainly used in the production of polyester, e.g., polytrimethylene terephthalate (PTT), as well as the synthesis of pharmaceutical intermediates. The microbial anaerobic fermentation is an efficient and environmentally friendly process as opposed to the traditional ethylene oxidation and acrolein hydrolysis, however, the optimal operating point with the highest product concentration is unstable. This paper introduced the washout filter-aided controller which was originally used for electric power system and aircraft to adjust the dynamic behavior of the anaerobic fermentation process. By selecting appropriate controller parameters, Hopf points were introduced near the optimal operating point to make the unstable optimal operating point stable in the closed-loop system without affecting the equilibrium manifold. Finally, simulations of the closed-loop systems were used to verify the effectiveness of the proposed method of adjusting dynamic behavior.

[334]

Modelling and Simulation of Pressure Swing Adsorption (PSA) Processes for post-combustion Carbon Dioxide (CO2) capture from flue gas

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Pressure swing adsorption (PSA) and vacuum swing adsorption (VSA) are gas separation processes which have attracted increasing interest because of their low energy requirements as well as low capital investment costs in comparison to the traditional separation processes. Hence, the development of optimization strategies for the design and operation of simple and complex PSA/VSA processes are of great importance in improving process performance.

A modelling framework for the separation of carbon dioxide (CO2) using multibed PSA/VSA flowsheets has been developed. The core of the framework represents a detailed adsorbent bed model relying on a coupled set of mixed algebraic and partial differential equations for mass, heat and momentum balance at both bulk gas and particle level, equilibrium isotherm equations and boundary conditions according to the operating steps. The adsorbent bed model provides the basis for building a PSA/VSA flowsheet with all feasible bed interconnections. The framework provides a comprehensive qualitative and quantitative insight into phenomena that take place in the process. The modelling equations have been implemented in the gPROMS modelling environment. We present the development of a modelling framework for efficient simulation and optimization strategies for the design of PSA/VSA processes with detailed adsorption and transport models. The modelling framework has been applied on the capture of post-combustion CO2 from dry flue gas.

We have also conducted a validation study of the above developed modelling framework against experimental and simulation data available from the literature. Validation studies included modelling of PSA/VSA processes concerning the separation of CO2 from dry flue gas. The simulation results of this work in terms of process performance indicators (CO2 purity, CO2 recovery and N2 purity, N2 recovery) are in good agreement with the data available from the literature. Furthermore, a systematic parametric analysis provides significant insight into the most critical design and operating parameters, and their effect on the process performance indicators. The parametric studies performed in this work have been carried out only in cases when it was necessary to clarify the effect of certain parameter on the process performance. Thus, once the base case parameters have been selected, only one variable at the time has been varied, and its effect analyzed. We have conducted a sensitivity study to determine which properties are most important in order to improve process performance.

Finally, we have also considered step-change perturbations in the feed flow rate to determine the response of a PSA/VSA process to feed disturbances. The perturbation effects are more pronounced in the first cycle after the perturbation, which allows the development of a control strategy with a very fast response to changes. After the last cycle of perturbation the CO2 gas phase concentration profile and the temperature profile tend to the cyclic steady state.

[359]

Validation of a functional model for early integration of safety issues into process system design

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A lack of general acceptance of a qualitative modeling paradigm for process systems has limited process system engineers in developing effective tools for handling issues related to Process Safety.

A qualitative functional modeling environment can accommodate different levels of abstraction for capturing knowledge associated with the process system functionalities as required for the intended application. Such a modeling methodology provides an effective means for solving a variety of PSE problems including behavioral attributes of system operation such as human error interaction with system operation. Therefore qualitative modeling is well posed to expand the existing capabilities in PSE modeling toolbox which predominantly relies on first-principles based mechanistic and quantitative modeling tools used in various PSE domain applications. This contribution focuses on an important aspect of model development, which is model validation. As it happens, a scientifically based validation method for functional models is missing and remains to be developed.

In this paper, two functional modeling frameworks are identified including object-centered view of function and teleological-oriented view of function. The former framework understands functional description as input-output relationship of black box, such as Function block diagram (FBD). The latter framework understands functions as a set of temporal events in sequence acted to achieve an intended goal. These two frameworks may lead to the two different practices on certain PSE tasks, i.e., design and analysis of safety systems in the early project development phase. The latter framework is emphasized in the paper due to the increasing interest. The Multilevel Flow Modeling (MFM) methodology is introduced in the framework. The validation aspects introduced through the means-end concept involves both validation of the goals as well as validation of the process functionalities. While the latter is well established for quantitative models the former requires a novel approach within process systems engineering. A procedure for validation of a functional model is proposed. Two modeling purposes are categorized: external modeling purpose and internal modeling purpose. To validate external modeling purpose is to ascertain whether the intended purpose is a relevant proposal. To validate internal modeling purpose is to ascertain whether the model implements the assumptions correctly, where the assumptions whether are reasonable in the given context relevant for both modeling purposes. With the reasoning capability provided by the MFM syntax and semantics, the validation procedure is illustrated on a simple engineering system (i.e. a heat exchanger system) of a MFM model with the external modeling purpose to meet the safety requirements early in the system design.

[370]

A Dynamic Method for Computing Thermodynamic Equilibria in Process Simulation

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In process simulation, a large variety of thermodynamic equilibria, such as reaction equilibria and phase equilibria between two or more phases, have to be solved in the different process units. It is common, that for different types of equilibria, different mathematical models are applied. For reaction equilibria, the most common approach is the Gibbs energy minimization method which formulates the equilibrium condition in terms of an optimization problem, i. e. minimizes the Gibbs energy of the system, see [1, p. 556]. In the case of phase equilibria, such as vapor-liquid equilibria (VLE) or liquid-liquid equilibria (LLE), a set of algorithms is available, that solves the equilibrium conditions, i. e. a set of nonlinear algebraic equations, directly, see [1, p. 245, 283] and [2].

In this contribution, we present a generalized approach for solving reaction as well as phase equilibria by solving a set of ordinary differential equations (ODE)

Here, A is a matrix which accounts for the stoichiometry of reaction as well as phase equilibria and r is a vector of thermodynamically consistent rate expressions that describe the fluxes between phases and/or fluxes due to chemical reactions.

An ODE system describes the evolution of the composition n of a given system w. r. t. time τ. It can be shown, that the steady state of this system corresponds to the thermodynamic equilibrium, i. e. fulfills the equilibrium conditions. The main advantage of the proposed approach, compared to conventional equilibrium calculations, is the fact that the ODE system always converges towards the thermodynamic equilibrium regardless which initial composition is chosen. We will demonstrate this advantage by considering and analyzing several examples of different complexity including systems with multiple reactions, multiple phases (VLE, LLE, LLLE) and also combined reaction and phase equilibria. Systematic comparison with established algorithms will be performed with respect to convergence, initialization, computational costs, and embedding into process simulation.

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[373]

Modelling and simulation of an enzymatic catalyzed reactive dividing wall column

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One of the major goals of process engineering is to improve the energy efficiency of industrial processes and therefore save energy costs and reduce emissions. Process integration makes it possible to reduce the energy as well as the investment costs. In the last years the concepts of reactive distillation and the dividing wall column have been subject of intensive research and also been implemented on an industrial scale. The reactive dividing wall column (RDWC) combines the two concepts creating a whole new piece of highly integrated equipment. Reactive dividing wall columns allow the simultaneous execution of a chemical reaction and distillative separation into three or more fractions. The advantage of using enzymes as catalyst is a high selectivity combined with high reaction rates at low temperature levels. However the high level of integration leads to a complex design process that requires suitable and reliable simulation models. In order to win the trust of companies to realize a reactive dividing wall column on an industrial scale the mathematical models need to be validated by experimental results.

Our research focuses on the modelling, simulation and experimental model validation of RDWCs. It is based on a model system: the heterogeneously catalyzed trans-esterification of butyl acetate and hexanol. After successfully developing and validating a rigorous mathematical simulation model for chemical catalyst trans-esterification, based on the concept of equilibrium stages (using experiments with our own pilot plant scale RDWC), we take RDWC research a new step forward. For the first time, a rigorous mathematical simulation model was developed for an enzyme catalyzed reactive dividing wall column, using the validated model for chemical catalyst trans-esterification as a basis . The model can be used for simulating reactive as well as non-reactive dividing wall columns with chemical or enzymatic catalyst. This allows an easy comparison between different types of catalyst. Additionally important input parameters for the simulation have been determined by our own extensive experiments. The calculation of the separation is based on experimental measurements of the vapor liquid equilibrium of the system for the pressure range from 30 to 900 mbar. The calculation of the reaction rates are based on measured chemical kinetics of the enzyme catalyzed reaction.

The presentation will contain three parts. The first part will give a short introduction into the concept of an enzyme catalyzed reactive wall column. The development from reactive distillation and a dividing wall column to the reactive dividing wall column will be shown and the difference between chemical and enzyme catalyzed reaction will be explained. The second part will cover the mathematical model. It will give an insight into modelling reactive dividing wall columns. Furthermore it will be shown which experimental data are necessary to model the separation process and the trans-esterification. The final part will show simulation results based on the model and the experimental measurements of reaction kinetics and vapor liquid equilibria. Especially the results for chemical and enzymatic catalyzed reactive dividing wall columns will be compared.

[403]

Co-production of butanol, acetone and electricity in an advanced biorefinery under a consolidated bioprocessing approach

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Conventional biorefineries based on biochemical platforms requiring enzymatic or microbial hydrolysis commonly involve three biologically mediated transformations (BMT): the production of saccharolytic enzymes, the hydrolysis of carbohydrate components in pretreated biomass to monomers and the fermentation of pentose and hexose monomers. Simultaneous execution of chemical reactions is a common strategy in process engineering. In biotechnologic areas, the simultaneous execution of these BMT in a single unit is known as Consolidated Bioprocessing (CBP). CBP has been considered as an alternative for biorefineries design since enzyme purchase is discarded and the number of stages and equipment needed for the substrate transformation decreases. However the techno-economic viability of CBP needs to be analyzed from a process engineering point of view. This work presents an advanced biorefinery scheme under a CPB approach for the ABE process. This scheme does not require a thermochemical pretreatment stage and simplifies the reaction stages which could lead to a total production cost (TPC) for butanol similar to an oil based process scheme.

A conceptual design is presented for the advanced biorefinery under a CBP approach. The scheme is conformed by six stages: (i) conditioning (milling and fibers hydration), (ii) dark fermentation (hydrogen production), (iii) methanogenic production (biogas production), (iv) ABE fermentation (acetone, butanol and ethanol production), (v) downstream processes and (vi) cogeneration. A non-conventional separation stage (downstream processes) is adopted from the literature consisting of an extractive-column train using mesitylene as the solvent extractor followed by a series of distillation columns. Wheat straw (WS) was used as feedstock for a plant capacity of 2,200 MT DB/day, analyzing the impact of the butanol concentration and the hydraulic retention time (HRT) on the TPC of butanol. Butanol concentrations (9.95, 15 and 19.4 g/L) and HRTs (8, 24, 40 and 72 h) were fixed based on previous studies utilizing different species of Clostridium. The operating conditions for each reactor (temperature, solid load, HRT and inoculum) were taken from previous published results and compared against our own experimental data. The steady mass and energy balances as well as the economic evaluation using the Net Present Value (NPV) technique were performed using SuperPro Designer v8.5. The results showed that in the best case scenario (8 h, 19.4 g/L), the butanol TPC was $1.17 USD/kg, also the cogeneration stage produces the needed energy for the biorefinery and a surplus electricity that could be distributed to the public electricity grid. The results showed that the butanol concentration had greater influence over the butanol TPC than the HRT. Details of the CBP biorefinery model as well as of the results obtained will be presented in the paper, together with a discussion on the advantages and drawbacks of using this process approach as an alternative to the conventional oil-based ABE process.

[406]

Retrofit of concentration plants using global sensitivity analysis

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This work presents the use of global sensitivity analysis to retrofit mineral concentration plants. The ore that is fed to a concentration plant is heterogeneous and it changes over time as the mine is operated. Moreover, the costs and the selling price of the concentrate can undergo significant changes. This situation forces readjust mineral concentration plants to the new conditions.

The Sobol's method is used to identify the variables that most significantly affect the recovery of the species and the grade of the final concentrate. The methodology is applied to a copper and molybdenum concentrator plant of three concentration stages. The models used to represent each stage were adjusted using plant data. The species present in the mineral correspond to Chalcopyrite, Chalcocite, Covellite, Molybdenite, Pyrite, and Quartz. Because the objective of the flotation circuit is to obtain a concentrate rich in Cu-Mo, the influence of the input factors on the variability of the grade and recovery of Cu and Mo in the final concentrate (output factors) is analyzed. The input factors correspond to 47 variables including the kinetic constants of the species in each stage, residence times and number of cells in each stage of concentration, solids concentration at each stage, among other variables.

The sensitivity analysis based on Sobol's method determines the factor inputs that generate more variability on the concentrate grade and recovery of Cu-Mo obtained in the flotation circuit. This analysis allows to significantly reducing the number of input factors on which to focus when a certain metallurgical objective is searched. Examples are used to show the validity of the results.

[412]

Differential-Algebraic Approach to Solve Steady-State Two-Phase Flow Drift-Flux Model with Phase Change

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Two-phase flow in pipes occurs frequently in petroleum refineries. Simulation and design calculations for their processing units require methods for predicting void fractions and axial pressure drops, thus making it essential that precise models of the relevant thermo-fluid dynamics be combined with efficient numerical techniques. In this work, the two-phase flow with phase change problem of a refinery multicomponent naphtha (C5-C8) was modeled through the steady-state one-dimensional mixture model, which comprises continuity, momentum and energy differential equations for the mixture, in addition to an extra continuity equation for the vapor phase. Relative motions between the phases are accounted for by a constitutive expression for the one-dimensional drift velocity. Evaporation and condensation are considered via vapor-liquid equilibrium calculations, and suitable thermodynamic methods are also applied in the evaluation of physical properties. It is proposed in this work that this rigorous formulation fits in the scope of Differential-Algebraic Equations (DAE) systems and is preferably solved by proper established numerical methods rather than the customary iterative segregated semi-implicit algorithms based on finite volume approaches. Efficiency and accuracy gains are demonstrated as a result of the proposed numerical strategy, which yields higher-order numerical solutions in much less CPU time. Specific regularization functions were also developed in order to eliminate expected numerical issues of convergence failure due to discontinuities in the drift-flux parameters at flow-regime transitions.

[433]

Model-based design of experiments for the identification of kinetic models in microreactor platforms

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Microreactor platforms represent an ideal system for the study and determination of intrinsic reaction kinetics for strongly exothermic, endothermic, and fast catalytic reactions. These systems allow these reactions to be performed isothermally and in the absence of mass transfer limitations, ensuring the rapid manipulation of reaction conditions and the precise control of the hydrodynamic environment [1]. However, the quantity, quality, and speed of information generation from microreactor platforms is strongly related to the experimental conditions realised during the trials. Model-based design of experiments (MBDoE) techniques [2] have been proposed in the literature for the purpose of designing a set of experiments yielding the most informative data to be used for model identification. Experiments can be designed for discriminating between candidate kinetic models [3] or, if a suitable model structure is available, to improve the precision in parameter estimation. Whilst the first objective is achieved based on the maximisation of the discriminating power, the second is based on the maximisation of the expected information given as a measurement function of the Fisher information matrix.

In this paper, a new procedure suitable for the optimal design of experiments in microreactor platforms is proposed which is articulated into three main steps: i) given a set of candidate kinetic models, a ranking of the available experiments is realised from parameter estimation in order to the detect both the experimental regions yielding the maximum amount of Fisher information and the ones providing the maximum discriminating power; ii) information maps are detected and used for the optimal design of experiments where the trade-off between Fisher information and discriminating power can be quantitatively evaluated; iii) the optimally designed experimental conditions are implemented in the microreactor system, providing new experimental data to be used for model identification. The repetitive iteration of steps i) to iii) lead to the detection of the best model structure representing the system, elucidating the most probable kinetic mechanism for a given catalyst, ensuring, at the same time, a precise estimation of the model parameters. The proposed procedure is tested on a real case study concerning the identification of kinetic models for the oxidative dehydrogenation of methanol to formaldehyde on silver catalyst. Experiments are carried out on a specifically designed microreactor fabricated in silicon by etching and where the silver catalyst was deposited by sputtering. The temperature, pressure and volumetric flow rate are controlled and continuously monitored; concentrations are analyzed online at the inlet and outlet of the microreactor using a gas chromatography system. The experiment setup offers the possibility to integrate instrumentation and automation algorithms for online optimisation.

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[447]

Application of Derivative-Free Estimator for Semi Batch Autocatalytic Esterification Reactor: Comparison Study of Unscented Kalman Filter, Divided Difference Kalman Filter and Cubature Kalman Filter

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The online or real time optimization system required an on-line monitoring for important state variables and parameters in order to provide feedback to the algorithm implemented. The unmeasured states and unknown parameters can be determined by estimator. However, the estimator may be bias if model uncertainties occur. Although the estimates are continually corrected in response to measurement, they are also continuously influenced by the incorrect model and thus will become incorrect. Model uncertainties may even cause the estimation errors to grow exponentially. Furthermore, disturbances that enter the process on-line can also introduce biases in the estimates. Consequently, the feasible estimator must have several functionalities such as bias-free parameter and state estimates, high speed of convergence from initialization errors, perfect tracking and short computational time. The most common way of applying the estimator to a nonlinear batch system is in the form of the extended Kalman filter (EKF). Nonetheless, EKF suffers several flaws that may seriously affect its performance. One of the flaws is the computation of the state transition matrix which calls for calculation of the Jacobian matrix and its matrix exponential, which, in turn, requires linearization of the system model. To address those issues, the derivative free stochastic observer is applied in this work. Different derivative-free techniques implemented which are based on the Gaussian approximation are scaled Unscented Kalman Filter technique (sUKF), Divided Difference Kalman filter (DDKF) and Cubature Kalman filter (CKF). Here, an autocatalytic esterification of Propionic Anhydride with 2-Butanol is considered as a case study. The performance of estimator which is indicated by the accuracy, speed convergence and robustness, is represented by the root mean squared error (RMSE). While, the efficiency of the estimator's computation are evaluated by CPU time consumed. The derivative free-estimators are then evaluated within three case studies which are normal condition, effect of disturbances and effect of uncertainty of initialization parameter. The results of overall state and parameter estimator study show that the CKF outperform the sUKF and DDKF for most cases under consideration. Moreover, computational load consumed for the CKF is feasible for online practice However, in term of CPU time DDKF results to the shortest among all techniques implemented.

[453]

Modeling and parameter estimation of coke combustion kinetics in a glycerol catalytic conversion reactor

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A two dimensional, heterogeneous model was developed for the simulation of a coked catalyst regeneration fixed-bed reactor in a green acrylics process. A kinetic model which consists of combustion of coke containing carbon, hydrogen and oxygen was derived. The unknown parameters (including the kinetic parameters, initial composition and concentration of coke, heat transfer parameters and catalyst pore diameter) were identified using the results of regeneration experiments with the coke formed in a glycerol dehydration process. Good agreements between the model predictions and experimental results were obtained.

[465]

Behavior of heavy metals during gasification of phytoextraction plants: thermochemical modelling

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Wastes such as contaminated biomass are widely available resources which could be gasified to produce syngas biofuels and electricity and thus help to cope with fossil fuel depletion and reduction of greenhouse gases emissions. However, contaminated biomass is used to a very small extent as a source of energy due to its potentially high content of heavy metals. As exemplified by the specific case of phytoextraction plants, which are used to extract contaminants from polluted soils, heavy metals accumulate inside the roots, stems and leaves of these plants. A thorough understanding of their behavior during gasification is thus required.

Recent works have shown that these heavy metals can have a significant influence on the kinetics and the thermodynamics of the gasification reaction. Indeed, depending on their nature, heavy metals have a catalytic or inhibitory effect on the conversion reactions. Since kinetic studies focused on thermochemical conversion of biomass and waste are more widely studied in the literature than thermodynamic aspects, the present work is focused on the modeling of thermodynamic equilibria during the conversion, which represent an important scientific challenge for optimizing the conversion processes. This thermodynamic model aims at predicting the reaction yields and the physical states of the products as well as the composition and speciation of the different phases, gas, liquid(s) and solids.

The model has been developed using a non-stoichiometric method, often referred to as "Gibbs free energy minimization approach". Its main advantage is that no chemical reaction needs to be given as an input to find the solution. For this purpose, the Equilibrium module of the FactSage thermochemical software has been used, thanks to its adapted capacities in the field of complex chemical equilibria and process simulation and the large compound database available.

The biomass considered in this study is willow, which is the most used plant in phytoextraction. Apart from major wood components (C, H, O, N), a large amount of contaminants has been taken into account: alkaline and alkaline earth (K, Na, Ca, Mg, Sr), heavy metals (Cr, Cd, Cu, Pb, Ni, Sn, Fe), light metals (Al, Ti, Mn, V), as well as B, Si, S, P and F.

As thousands of compounds and phases exist in the multicomponent system composed of contaminated willow, a preliminary selection of the compounds which might form in gasification conditions was established. The selection procedure, based on the systematic calculation of predominance diagrams, lead to the establishment of a specific database containing a few hundreds of compounds. Then, depending on operating conditions (temperature, pressure, solid/gas ratio), equilibrium calculations allow to discuss the composition of gas, liquids and solids produced from the gasification of contaminated willow, with a specific focus on the behavior of the heavy metals. A clear picture of the most stable compounds is provided.

On-going work is furthermore aiming at developing a kinetic model based on experimental data, in order to compare the thermodynamic calculation with experimental tests and improve the understanding of reactions taking place during contaminated biomass gasification.

[467]

Multi-objective optimization for the production of fructose in a Simulated Moving Bed Reactor

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The isomerization of glucose into fructose is an important reaction for the food industry. Fructose based syrups compete with sucrose (from cane sugar) in many food applications as sweetener. Fructose is 2-3 times sweeter than sucrose - which means basically that less raw material is required to give taste to for example soft drinks and that makes the production cheaper. As a result the change in world prices of cane sugar dropped and basically crippled sugar economies.

However, more recently the isomerization reaction of glucose into fructose was also proposed as a new means towards the bio based economy. Fructose is the starting material for the synthesis of furancic precursors which can be used to produce non-petroleum derived polymers. In addition, glucose is a monomer unit of the abundantly available polysaccharide cellulose. Glucose has the potential to become the most important organic raw material for a society depending on biomass recourses.

The big challenge exists in the separation of the formed product from the reaction mixture. The separation of isomers and other similar components is generally performed in a chromatographic/adsorption separation system. These systems are operated in a non-continuous fashion. The isomerization reaction can be combined with the adsorption reaction into a simulated moving bed reactor. The introduction of the simulated moving bed reactor makes it possible to perform reactions and chromatographic separations quasi-continuously. Moreover, since the reaction is reversible, the combination of reaction and separation intensifies the process by shifting the equilibrium. It is, however, difficult to optimize the design and operation of a simulated moving bed reactor due to the many variables and the cyclic nature of the process.

In this work, a MATLAB model is developed for the simulation of a simulated moving bed reactor with 4 and 8 columns. The model with 4 columns is optimized for maximal throughput and product purity in the separation of glucose and fructose.

Optimal operation parameters are reported for various purity requirements, which show that a simulated moving bed reactor with 4 columns can best be operated with a feed velocity of 8.58 m=h at which purities of 92.9% and 80% are achieved for the fructose and the glucose product. For the SMBR with 8 columns, the optimal feed flow is 10.62 m=h, at which purities of 96.3% and 84.8% are achieved for the fructose and the glucose product streams.

Ultimately we use multi-objective optimization to balance the product purity with the product throughput by generation of a pareto front of non-inferior solutions. By using Pareto approach we measure the solution that is closest to the Utopia point and propose this as best solution to the problem.

[502]

A modeling framework for optimal design of renewable energy processes under uncertainty

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In recent years there has been a marked surge in the search for alternative sources of energy that wean the world off of dependence on fossil fuels and reduce the carbon foot-print. As the world has recognized the importance of diversifying its energy resource portfolio away from fossil resources and more towards renewable resources such as biomass, there arises a need for developing strategies which can design renewable sustainable value chains that can be scaled up efficiently and provide tangible net environmental benefits from energy utilization. After a boom in U.S. corn-based ethanol in the early part of the 21st century, the interest has gradually shifted towards more viable sources of biofuels and biochemicals. Second generation biofuels are examples of such fuels that are extremely attractive owing to the fact that the raw materials can be composed completely of "left-over" wastes of food crops and forest harvests that don't interfere with the human food chain and the natural ecosystem. It also can provide new income and employment opportunities in rural areas. Further, due to the large variety of lignocellulosic materials and their abundance, these types of produced fuels and chemicals can overcome the challenge of limited feedstock availability that first generation biorefineries have to contend with.

In this study we present the development and implementation of a multi-layered decision support tool for the optimal design of renewable energy systems under the presence of uncertainties. We apply a distributed, systematic approach which is composed of different layers including strategic, tactical, and operational tasks. To demonstrate the effectiveness of the proposed methodology, a hypothetical case study of a multiproduct lignocellulosic biorefinery based on sugar conversion platform is utilized.

Linear programming (LP) models are suggested for the purpose of strategic planning. To overcome the mismatch between nonlinear process mechanisms and LP-based strategic optimization, a decomposition strategy is proposed that combines net present value (NPV) optimization for long term planning with rigorous non-linear process simulation and process-level optimization. Different scenarios are developed based on stochastic forecasts for uncertain market parameters including price and demand of bioproducts. The process is formulated as a mixed integer linear programming (MILP) model which incorporates a stepwise capacity expansion strategy by defining binary variables for capacity increments at each time period in the planning horizon instead of establishing the whole capacity during the first planning year. The output of the model includes optimal design of production capacity of the plant for the planning horizon by maximizing the net present value (NPV). Then this capacity is sent to the lower level of the optimization algorithm. The second stage, which optimizes the operating conditions of the plant, consists of three main steps including simulation of the process in the simulation software (nonlinear modeling), identification of critical sources of uncertainties through global sensitivity analysis, and employing stochastic optimization methodologies to optimize the operating condition of the plant under uncertainty. The proposed methodology has the advantage of being able to integrate long term planning based on financial optimization with nonlinear process mechanisms, and also optimize process operating conditions under the presence of uncertainty.

[504]

A molecular reconstruction feed characterization and CAPE OPEN implementation strategy to develop a tool for modeling HDT reactors for light petroleum cuts

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Hydrotreating is a process widely used in the petroleum industry for producing high quality fuels and as part of a scheme for upgrading heavy crude oil. In this work, the hydrotreating of light petroleum cuts with a boiling point range between 390-670 K was taken as case of study to develop a model that represents this process. Initially, a molecular reconstruction approach based on the entropy maximization criteria was applied to model the feed, where a set of pre-defined molecules and the main operational variables that characterize it were taken into account to pose the mathematical formulation of the reconstruction. The reactor was modeled using a trickle bed representation, considering the following reactions in the kinetic formulation: hydrodesulphurization (HDS), hydrodenitrogenation (HDN) and aromatic hydrogenation (HDA). Kinetics for each reaction was modeled as follows: HDS with the Langmuir-Hinshelwood approach, HDN as a direct reaction described by a first order power law kinetics and HDA as a first order reversible reaction. The reactor model considers complete wetting of the catalyst surface so only reactions in the liquid phase are modeled. Rigurous phase equilibrium calculations were made in order to calculate the component concentrations in the gas-liquid interphase along the reactor length. The validation data was generated under pilot plant test conditions at constant pressure, LHSV and hydrogen/feed relation of 8*106 Pa, 1,2 h-1 and 700 Nv/v respectively. Temperature was modified from 580 to 610 K. Finally, the model was implemented as an interoperable software component based on the CAPE OPEN standard, where a dedicated thermodynamic package was used to calculate rigurously all the properties and phase equilibria estimations required to carry on the calculations into the reactor model. Results were found in good agreement with experimental data.

[506]

Dynamic Modelling and Experimental Validation of a Pilot-Scale Tubular Continuous Reactor for the Autohydrolysis of Lignocellulosic Materials

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The pretreatment of lignocellulosic materials (LCM) is one of the most important steps in the production of biofuels and sugar-based products using biochemical platforms. If the LCM is not properly processed at this stage, the yield and performance of down-stream stages (e.g. enzymatic saccharification, fermentation and purification) may be seriously affected. Among pretreatment methods and technologies, autohydrolysis is considered a very promising alternative due to its lower environmental impact and operating costs and less operational complexity.

This work focuses on the dynamic modelling of a pilot-scale tubular reactor (PTR) used for the pretreatment of LCM. The PTR works in three phases: first the LCM is fed by a system of pistons into the reactor, in an extrusion process, then a thermal hydrolysis stage takes place in the tubular body of the reactor, and finally, the LCM is expelled from the reactor by a "steam-explosion" step. In this case, the LCM consists of grinded wheat straw, and is heated with saturated vapor at 90 psi (433 K).

The proposed model describes the reactor dynamic behavior during the second phase (autohydrolysis), and is based on a non-isothemal first order kinetic model that describes the wheat straw thermal hydrolysis process. This model takes into account the production of intermediate oligosaccahdies as well as the contribution of aceto-compounds in the reaction rates. The PTR was modelled as an arrangement of four Continuous Stirred Tank Reactors (CSTR) in series, in order to have an equations set with the residence time (τ) as an explicit variable, where τ can be used as an input variable in the associated control scheme. The model performance was validated with experimental data including concentration profiles of hemicellulose, cellulose, glucose and xylose in the PTR outlet stream, as well as the temperature and acidity profiles.

The proposed model is able to describe the dynamic behavior of the reactor at 433 K, within reasonable tolerances. Nonetheless, at these operating conditions, the extrusion and "vapor-explosion" phases, offers little or no contribution to the pretreatment process, leaving the overall performance to the autohydrolysis phase.

[507]

Techno-economic analysis of ethanol-selective membranes for corn ethanol-water separation

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Currently, three distillation columns are used to separate ethanol from water in traditional dry-grind corn ethanol facilities. Corn ethanol production by fermentation with yeast in the U.S. is approximately 13.3B gallons per year. Ethanol forms an azeotrope with water at approximately 95wt% which makes the separation by distillation energy intensive.

Membrane separation by vapor permeation is not affected by this azeotrope and has the potential to significantly reduce the energy consumption of these facilities which would in turn reduce the overall operating costs of the facility.

The vapor-liquid equilibrium (VLE) of the ethanol water system has a distinctive bulge at lower (<50wt%) ethanol concentrations. This suggests that there is a large driving force for ethanol recovery in the vapor phase at lower concentrations. This is ideal for distillation columns. However, this driving force quickly reduces as the ethanol concentration approaches the azeotrope. The VLE diagram qualitatively suggests that a system that combines distillation followed by a membrane technology may be able to outperform a stand-alone distillation or membrane system.

In this work, we systematically study such a system. We model the existing technology in Aspen Plus in order to understand the base case performance and costs. The membrane unit is modelled in gPROMS as a zeolite based counter-current hollow fiber plug flow unit. This model is used to systematically investigate the process economics of a hybrid system which combines a distillation column and membrane unit. The final configuration involved a recycle of the membrane retentate to the distillation column inlet.

We investigate how the economics of these systems are affected by changes in key membrane performance parameters such as membrane flux, selectivity and costs. These sensitivity analyses allow us to determine the parameter space which allows for economically attractive commercialization of this membrane technology in dry-grind corn ethanol facilities.

[511]

Equation-oriented Modeling of Multi-stream Heat Exchanger in Air Separation Units

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Multi-stream heat exchanger (MHEX) is a process unit in which multiple hot and cold streams can exchange heat simultaneously. MHEXs are widely used in cryogenic systems which require recovery of huge cold energy at very small temperature driving forces, such as air separation and liquefied natural gas (LNG) units. Modeling technique of MHEX is particularly important to advanced control and real-time optimization of air separation units. However, a first principle model based on heat transfer encounters a challenge to well handle the nonlinear phase changes of streams. Moreover, it is very difficult to develop such a MHEX model without detailed internal structure information, which is sometimes unavailable due to the proprietary protection. In this project, a data-driven model with consideration of the general bundle structure is proposed. In air separation units, some streams often enter or leave an MHEX from a certain layer in the middle section. Complex MHEX is thus decomposed into several bundles which do not allow streams to enter or leave the equipment in the middle layer. For each bundle, a regression shortcut model is built to describe the effect of inlet temperatures and flowrates on outlet temperatures. Heuristics are also introduced to help determine the model structure. An equation oriented (EO) model can be eventually built by linking all bundles together. The simulation on this model requires solving equations simultaneously. By collecting a large number of operating data, the model can be obtained through optimization. To simplify the solving process, an initialization technique through sequential mode is also proposed. The case test shows the good performance of the proposed shortcut model with prediction error less than 2%. Finally, the method is applied to a commercial 20000 Nm3/h internal compressed air separation unit.

[524]

Superstructure Development, Simulation and Optimization of Desalination Systems using Aspen Custom Modeler

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Since the demand of clean and potable water has exceeded its supply in many countries, numerous studies have been invested in desalination to search for viable, economical and sustainable processes to produce freshwater from sea and blackish water for domestic, industrial and other applications. Over the last two decades Reverse Osmosis (RO) and Multistage Flash (MSF) have become two of the leading technologies in the desalination area. New ideas of combining and/or switching between RO and MSF in a hybrid system have also been investigated. The so-called hybrid desalination systems have been proved to improve water quality while reducing energy consumption and/or operating cost, but they have not been tested yet on an industrial scale and there is limited research work done on the modelling and optimization of these systems.

RO and MSF are two different techniques; RO uses membrane while MSF uses thermal technologies. However, these two can share common pre-treatment stages. Both processes are temperature-dependent, driven by pressure differences and can be designed as a single or multiple stage systems. In this paper, thermal (MSF) and membrane (RO) systems are modelled and simulated in Aspen Custom Modeler (ACM) V.8.4. The major advantage of using ACM is that a single stage mathematical model can firstly be developed for MSF and RO. Then, a multiple stage model can be easily built based on the single stage model by adding one or more modules. Both steady state models include material balances but RO focusses more on pressure differences while MSF relies on energy balances. Solving these models would require information such as water permeability for RO and top brine temperature for MSF. In this work such information would be obtained from the open literature to test the feasibility of the system.

After developing the individual MSF and RO models, the next step involves the development of the model of a hybrid superstructure by combining individual flow sheets of MSF and RO systems. The superstructure is used within an optimization framework to analyse and optimize various process configurations (including the number of stages). Operating conditions such as temperatures, pressures and process design variables such as membrane or heat transfer areas are used as optimization variables to minimise the economic objective function. Finally, the results of the superstructure optimization are presented and discussed.

[532]

Microalgae growth determination using breakage equation model

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Microalgae can be used for several purposes such as for production of biofuels, proteins and fine chemical extraction, without competing with land for crops. The production of biofuels from microalgae imply the need of growing the microphytes in photobioreactors. Algal growth in this kind of reactor is strongly affected by several environmental parameters such as temperature, light intensity, CO2 concentration in the liquid phase, pH and nutrients concentration. In order to build a growth model for microalgae all these parameters shall be considered.

When measuring the growth of microalgae, besides the growth rate in total mass, the population density and size distribution, that are often neglected, can provide additional information on the growth condition and the accumulation of chemical components such as lipid inside the microalgae cells. This paper presents a novel growth model of microalgae taking into account its population growth cycle. A population balance model with breakage equations, typically used in crystallization for evaluating the particle size distribution (PSD), is adapted. The variations in PSD is an important information for knowing the microalgal health conditions. The proposed model also take into account the death of microalgae caused by dense population or poisoning triggered by the dead microalgae or poor growth conditions. The model is experimentally verified. Results from the model can be used for improving the production process or to maximize a desired component inside the microorganisms. With the predicted population distribution, we could determine the timing or design suitable method for harvesting, adjusting nutrient levels, etc. The model can generally be used for various biological systems.

[536]

A new strategy for the simulation of gas pipeline network based on system topology identification

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Pipeline network plays a very important role in chemical plant, refinery, oil and gas gathering. Design, optimization and scheduling of pipeline network are based on the simulation of pipeline network. Pipe segment is defined as basic unit in pipeline network. Different pipe segment has different pipe length, pipe diameter. Every pipe segment can be described by a flow-pressure nonlinear equation including flow, pressure, pipe length, pipe diameter, Fanning factor and density. With the increase of number of pipe segments, the number of variables and equations increases sharply, therefore, the corresponding relationship between flow rate and pressure is strongly coupled across the network. Pipeline network model becomes more difficult to be solved. Different from liquid, gas is compressible fluid, which means gas density is also a variable in this system. This will increase the difficulty of solving the pipeline network model. Currently, there are two methods for solving pipeline network. One is sequential modular method; the other is equation oriented method. It is difficult to find correct order to solve pipeline network by sequential modular method. Thus nonlinear equations need to be calculated by equation oriented method. However, this method has large computational complexity and it highly depends on initial values. When there are more unknown variables, it is hard to assign an appropriate initial values and also hard to get convergence. In this work, a pipeline network model suitable for compressible gas is built. The simulation of a pipeline network with compressible fluid are decomposed to the identification of the pipeline network topology and the equivalence of pipeline network into several simple pipeline networks. Pipeline network topology can be described by adjacency matrix. Pipeline network topology identification can be achieved by adjacency matrix searching, by which pipeline network model is simplified to the combination of equivalent sub-network of pipeline. This adjacency matrix searching process is actually the process of simplifying equations. After the simplification, the number of equations is reduced and gas pipeline network model is therefore easier to solve. In our work, this solution is applied to an actual gas pipeline network for verifying the model and solution proposed in this paper.

[551]

Modelling and optimization of a heat integrated gasification process

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Equilibrium modelling of the gasification process is widely utilized in process studies and has satisfying estimation of syngas composition. Recently, it is reported that the equilibrium modelling which took residual carbon into consideration predicted gas composition more accurately. However, how the operating parameters such as oxygen ratio, gasification temperature etc. would affect the carbon conversion and subsequently cold gas efficiency (CGE) as well as gas yields is seldom studied systematically.

In the present study, the equilibrium model based on Gibbs free energy minimization is developed to study the characteristics of carbon conversion in a gasification process. The effects of oxygen-to-carbon ratio and other gasification variables on the carbon conversion efficiency, CGE and product yields are discussed. In order to estimate the yield of both gaseous products and residual carbon, a multiphase formulation of which Gibbs free energy of solid carbon along with the gas mixture is included in the model. This allows the carbon conversion to be quantitatively analyzed.

Initially, the proposed model is applied in the oxygen gasification and oxygen-water gasification. Addition of water helps the gasification enjoy low-temperature requirements for refractory materials and higher CGE due to the water related endothermic reactions and improvement of the carbon conversion efficiency. The higher heating value (HHV) of the wet syngas ranges from 13.80 to 15.50 MJ/Nm3 in oxygen gasification while 12.12-16.39 MJ/Nm3 of syngas is obtained in oxygen-water gasification. Though the range of fluctuation expands, the benefits can be expected with well-controlled amount of gasifying agents. Also, the influence of gasification temperature on the carbon conversion efficiency is quantitatively analyzed through the heat addition and extraction. Furthermore, the parametric study of oxygen-water gasification is conducted by varying the amount of water added. It is found that the increasing amount of gasification feed water (GFW) shifts the complete conversion towards the lower oxygen-to-carbon ratio. The systematic study on influencing factors of carbon conversion gives insights of adjusting the gasification parameters including gasifying agents, gasification temperature etc. for better performance.

[555]

Analyzing and Modeling Ethylene Cracking Process with Complex Networks Approach

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This paper focus on understanding the ethylene cracking reaction (ECR) networks with complex networks approach to polish up the accuracy of the product prediction. Though the molecular reaction model, lumped reaction model, and radical reaction model which establish a kinetic scheme of the pyrolysis reaction from different aspects are introduced to numerical simulation of the n-alkanes pyrolysis process, construction and simplification of the reactions are still the important problem the scholars concerned most because of the paradox that a complete networks cannot have the property in a simplified network such as less computing time. To simplify the reaction network, the scientists apply some mathematic methods such as sensitivity analysis, principal component analysis (PCA) and computational singular perturbation (CSP) to analyze the reaction networks that have amount of nodes and connections in the graph.

The need to deal with a large number of reactions exactly draw our attention to the complex networks approach. Complex networks theories come from the graph theory with the computer revolution providing the scholars with a huge amount of data and computational resources to process and analyze these data. Furthermore, considering the real-world network characteristics, these theories have been widely used in understanding many networked systems from biology, computer science, engineering, etc.

In this paper, as the complex networks research has grown steadily for its potential to represent, characterize and model a wide range of intricate natural systems and phenomena, the method of statistical physics is applied to represent the topological structure of ECR network. Furthermore, the algorithm of graph detection assists us in searching the community structures of the ECR network with which the characteristics of the different types of reactions can be grasped. With the analysis of ECR networks, our model modifies the construct of cracking networks generated with detailed chemical radical reaction mechanism and numerical simulates the ethane and propane pyrolysis process in tubular reactor with the data from the lab. As a result, the product yield the model predicted shows a reasonable match with the experiment data.

[570]

Numerical analysis for mixing effect during particle coating process via twin screw extruder

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Twin screw extruder is one of the most important equipment for polymer molding or particle coating process because it has many advantages like solvent-free and minimum residue. In general polymer molding process, the fill ratio which represents the ratio of polymer to gas inside the extruder has maximum value (usually 1) at the kneading block zone so called mixing zone. So in the case of particle coating process, mixing of the particles with the polymer mainly takes place in the mixing zone. And usually the mixing zone includes many kinds of kneading elements of screw and they have different role for mixing. In this study, the mixing effect of the particles is calculated in different arrangement of several kneading elements and conveying elements. Six cases of elements arrangement in the mixing zone are assumed and every case have 100mm long total screw including 45mm long mixing zone. For calculating mixing effect inside the twin screw extruder, computational fluid dynamics (CFD) model was developed and flow pattern and dynamic behavior of operating polymer were analyzed. The CFD model includes the Power-Law viscosity model for data fitting of viscosity which is obtained experimentally and remeshing technique to investigate screw rotation situation as well as internal dynamic behavior of liquid polymer. To represents the mixing effect as numerically, Manas-Zloczower mixing index is introduced and to confirm the mixing effect, the motion of particles was observed when they were initially injected to twin screw extruder at two different positions of inlet: left and right side of inlet. Injected particles were colored differently by position: red and blue. In conclusion, mixing effect is strongly related to screw geometry and mixing index shows highest value at the perpendicular kneading block. This result is expected to be a good reference for modeling of twin screw extruders or designing of twin screw extruder particle mixing process.

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[571]

Optimization and Economic Evaluation of Bioethanol Recovery and Purification Processes Involving Extractive Distillation and Pressure-swing Adsorption

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Biofuels are an attractive source of renewable energy as they can easily replace liquid fuels used in transportation and many other types of machinery [1]. The use of renewables is gaining importance in view of depleting fossil fuel reserves and environmental concerns. More than half of the world's production of fuel ethanol comes from the U.S. and Brazil, where corn or sugar fermentation, respectively, is still the main process used for production. Publications in the last decade have focused mainly on amount of energy consumed per unit production of ethanol without regards to economic feasibility. In addition, there has been only one comparative study of extractive distillation to pressure-swing adsorption (PSA), where proper heat integration was not considered for the PSA process, hence resulting in an unfair comparison between different separation techniques [2]. The present study considers a 3-component feed of ethanol-water-CO2 from which ethanol is recovered and purified using 2 different techniques: 1) pressure-swing adsorption (PSA) with molecular sieves; and 2) extractive distillation with ethylene glycol (EG). The two processes are optimized considering CO2 content in the product, feed, recycle and side-draw stages, total number of stages, distillates, bottoms and side-draw purities, and feed temperature. Heat integration in both processes is also performed to ensure a fair basis for evaluation.

The present work is carried out systematically to assess the two recovery and purification techniques on a consistent basis. Both the processes are simulated and optimized using Aspen HYSYS v8.2. The entire downstream recovery and purification process is considered to allow better optimization of each separation technique employed. The processes are optimized to minimize unit production cost, which is a better indicator of the process feasibility for industrial implementation. Energy integration is implemented through pre-heating of feed with hot streams in the process and the use of mechanical vapor recompression, if applicable. Equipment design and specifications follow the guidelines provided in chemical plant design books. The advantages and disadvantages of each process are analyzed both qualitatively and quantitatively to identify the relative strengths of one process over the other. Our detailed and consistent study and its findings will be presented and discussed at the PSE2015/ESCAPE25 joint event.

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[583]

Data Reconciliation in Reaction Systems using the Concept of Extents

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Reliable kinetic models of chemical reaction systems should include information on all rate processes of significance in the system. Apart from chemical reactions, such models should also describe the mass exchanged with the environment via the inlet and outlet streams and the mass transferred between phases. Model identification and the estimation of rate parameters is carried out using measurements that are obtained during the course of the reaction [1]. Model identification often leads to the combinatorial complexity of identifying simultaneously all rate processes [1]. Alternatively, it can be carried out incrementally by transforming the concentrations to extents and identifying each extent separately [2].

Since measurements are inevitably corrupted by random measurement errors, the identification of kinetic models and estimation of rate parameters are affected by error propagation [3]. Data reconciliation is a technique that uses constraints to obtain more accurate estimates of variables by reducing the effect of measurement errors [4]. Data reconciliation can be formulated as an optimization problem constrained by the law of conservation of mass [5, 6] and positivity of reconciled concentrations. Consequently, model identification can be performed with reconciled concentrations. This paper presents a reformulation of the original reconciliation problem directly in terms of extents. This allows using additional constraints such as the monotonicity of extents. Such a reformulation improves the accuracy of the reconciled extents and hence of concentrations, and leads to better model discrimination and parameter estimation. The advantages derived from the use of reconciled extents are illustrated using a simulated example.

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[594]

Development of a ruthenium reactor generic model

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A mathematical first-principles model (FPM) of a ruthenium reactor was developed, implemented and successfully validated against a set of measurements of the real reactor at a precious metal refinery (PMR). The model describes the dynamic behaviour of a process involving two exothermic reactions, a dissolution and an evaporation, occurring simultaneously in a semi-batch reactor equipped with a jacket. As the reactor model grew to the final form presented in this paper, two versions of the model were developed as a result of the various numerical difficulties we had encountered during the modelling stage. The model was initially written as a set of fully implicit differential algebraic equations (DAEs), and generated incorrect numerical integrations. It was then reformulated in an equivalent system of explicit ordinary differential equations (ODEs), which was able to demonstrate satisfactory predictions of the real reactor behaviour. This version provided better accuracy in the model simulated variables of reactor temperatures and pressures in comparison to the measurements of the real ruthenium reactor.

[610]

First-principles model diagnosis in batch systems by multivariate statistical modeling

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Recently, a methodology has been proposed to diagnose the root cause of the process/model mismatch (PMM) that may arise when a first-principles (FP) process model is challenged against a set of historical experimental data [1]. The methodology refers to continuous systems and exploits a historical dataset of actual process conditions and a simulated dataset generated by the FP model using the same inputs as those of the historical dataset. A multivariate statistical model is used to analyze the correlation structure of the historical and simulated datasets, and information on where the PMM originates from (model equations or model parameters) is obtained using diagnostic indices and engineering judgment.

In this work we extend the methodology to the diagnosis of FP models of batch systems. As a test bed, a solids drying process, whose model is developed using gSOLIDS® [2], is investigated. Three different approaches to FP model diagnosis are developed and their performance compared.

In the first approach, a multi-way principal component analysis (MPCA [3]) approach is considered. To account for the diversity of the solid particle sizes, an appropriate transformation of the variables is introduced together with an orthogonal rotation (VARIMAX rotation [4]) of the MPCA model directions. This improves the information provided by the MPCA model residuals.

In the second approach, an estimation of the distribution function of the model residuals is done. This allows one to define more appropriate diagnostic indices that can be used also when the residuals obtained using the first approach show non-normal distributions [5].

Finally, a recently proposed fault detection methodology [6] is adapted to the PMM diagnosis task, exploiting the partial correlations coefficients of the variables analyzed. The approach is particularly useful to analyze and compare the changes in the correlation structure of the simulated and historical datasets, especially when the variables analyzed show strong and nonlinear relations.

The application of these different approaches shows the flexibility of the proposed methodology on treating data with different features and the ability to provide useful information on the reasons of a mismatch, even with complex batch processes.

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[625]

Integrated analysis of an evaporation and distillation bioethanol industrial system using direct and indirect heating

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Sugarcane processing is one of the most important and strategical sectors in the Brazilian economy. This important segment has steadily increased its activity in the last decades, propelling all sugarcane-related activities. It is expected that the 2013/2014 crop reaches 652 million tons, what in turn will suppose 27.17 billion liters processed in the ethanol distillation plants, a 15% increase compared to 2012/2013 [1].

In Brazil, ethanol is produced primarily from sugarcane juice. Sugarcane stillage (called vinasse), the final by-product of the biomass distillation, is rich in minerals and can be used for agriculture or animal feed. Vinasses are commonly used to irrigate sugarcane plantation, but if used in excess, may became an environment pollutant [2]. The low pH, electric conductivity, and chemical elements present may cause changes in the chemical and physical–chemical properties of soils, rivers, lakes and ground water, and may also have adverse effects on agricultural soils and biota in general [3].

In previous works [4], modeling, simulation, validation, and analysis of a sugarcane juice industrial evaporation system (IES) were performed. The IES included a falling film evaporator followed by three short vertical-tube evaporators operating in parallel. The model was developed using Hysys, a commercial process simulator, and their predictions were validated with operating data. The steam and juice stream flow rates predicted had a mean absolute difference of only 0.11%.

In this work we modeled, simulate, and integrate the system of evaporation, fermentation and distillation with direct heating. In addition, we proposed new scenarios using indirect heating in order to decrease the quantity of stillage, and consequently, minimize the environmental impacts associated. In this sense, a reboiler using the steam produced in the evaporators was included in the distillation column to analyse the effect of such revamping. Sensitivity analyses were performed to detect of key operational variables with effect on the process. The evaluation of the different alternatives developed allowed us to identify the best alternatives from both, economic and environmental perspectives.

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[627]

Reformulating the minimum eigenvalue maximization in optimal experiment design of nonlinear dynamic biosystems

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Dynamic bioprocess models provide valuable insight for the bioprocess industry in view of analysis, control and optimization of bioprocesses. After an accurate model structure has been determined (e.g., Stamati et al., 2014), parameter values have to be identified. Informative experiments are highly valuable for estimating parameters in nonlinear dynamic bioprocesses. Techniques for optimal experiment design ensure the systematic design of such informative experiments (Franceschini and Macchietto, 2008).

The E-criterion which is often used as objective function in optimal experiment design requires the maximization of the smallest eigenvalue of the Fisher information matrix. When optimization routines, which exploit gradient based methods, are employed, the E-criterion poses numerical challenges. The advantage of gradient based schemes is that they are fast and can tackle a problem with a large number of decision variables By construction is the Fisher information matrix symmetric and positive semidefinite. So, all eigenvalues are nonnegative real numbers but the minimum eigenvalue function can however be nondifferentiable. A second problem is that no closed form expression exists for the computation of eigenvalues of a matrix larger than a 4 by 4 matrix.

In the current paper a reformulation strategy from the field of convex optimization (Vandenberghe and Boyd, 1996) is suggested to circumvent the aforementioned difficulties. This reformulation requires the inclusion of a nonlinear matrix inequality constraint involving positive semidefiniteness. In the current paper, this positive semidefiniteness constraint is imposed via Sylverster's criterion (Wicaksono and Marquardt, 2013). As a result the maximization of the minimum eigenvalue function can be formulated in standard optimal control solvers through the addition of nonlinear constraints. These problems can also be solved using sequential semidefinite programming (Telen et al., 2014)), but require dedicated semidefinite program optimization routine. The presented methodology is successfully illustrated with a challenging case study from the field of bioreactor engineering.

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[634]

A Framework for Modular Modeling of the Diesel Engine Exhaust Gas Cleaning System

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Diesel engine exhaust gases contain several harmful substances. The main pollutants are carbon monoxide (CO), particulate matter, and nitrous gases such as nitrogen oxide (NO) and nitrogen dioxide (NO2). Reducing the amount of these substances is of great importance due to new legislation, and because of the effect they have on urban air quality. The exhaust gases are handled with four different catalysts: Diesel Oxidation Catalyst (DOC), Diesel Particulate Filter (DPF), Selective Catalytic Reduction Catalyst (SCR) and Ammonia Slip Catalyst (ASC). To be able to fully understand and optimize the system without using too many resources, it is necessary to be able to simulate the complete system under different scenarios. A modular model consisting of the different blocks representing the different catalysts would be able to simulate almost all diesel flue gas cleaning systems, and would therefore be a big help towards understanding the flue gas cleaning system and a step towards reducing emissions.

To achieve this, models of all the relevant catalysts have to be developed. The models have to be built in a way that they can work together, and since the dynamics play an important role in especially the SCR catalyst, all models should be capable of dynamic simulations. Kinetic models for the relevant catalyst reaction have to be gathered, and the kinetic parameters calibrated or gathered from literature.

Four different models have been independently developed with different purposes in mind. The reaction kinetic models, where relevant, have been gathered from literature. For the DOC, a channel model able to handle dynamic simulations has been developed, where the kinetic parameters have been found in literature. The model has been validated with data found in literature. For the DPF, a single-channel model has been developed capable of simulating some aspects dynamically. The data used for validation was collected from literature. The model for the SCR catalyst is a single channel model, where the kinetic parameter values have been calibrated using experimental data. The ASC model is a dual layer ammonia oxidation and SCR catalyst, considering steady-state scenarios. The ammonia oxidation kinetic parameters were calibrated with experimental data, and the SCR kinetic parameters were taken from literature.

Challenges with this project are to modify the models so that they can work together in a modular fashion, and also for the kinetics to be generic enough to work with different catalyst substrates. The goal is to explore if it is possible to take models that have been developed individually and for their own purposes, and use them to make a combined modular model.

[639]

An approximate modeling method for industrial L-lysine fermentation process

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L-lysine is an important chemical, usually produced by fed-batch fermentation process. Usually, feed stock compositions, reactant or product concentrations, and operating conditions vary with different fed-batches in this process. It is difficult to establish a kinetics-based model for an industrial fed-batch fermentation process. In this paper, we proposed a data-based approximate graphical modeling method to model this process. Variables values are treated as correlated Gaussian process. The methodology comprises of two important steps: i) the missing-data imputation within records, and ii) the dynamic Bayesian network learning, including structure learning, using the low order conditional independence method, and parameters learning, using the multivariate auto regressive method. The L-lysine fed-batch fermentation process is studied to demonstrate the effectiveness of this approximate modelling method.

[641]

Environmental and Economic Impacts of Biomass Pretreatment for Ethanol Production: Detoxification and Delignification Modeling

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Lignocellulosic biomass is the most promising feedstock in nature for the production of the so-called secong generation biofuels, considering its great availability and low-cost. Furthermore, these biofuels have the potential to replace first generation ones, thus avoiding the controversies resulting from the use of food crops for fuel production. Lignocellulosic materials contain a heterogeneous mixture of biopolymers from plant cell walls: cellulose, hemicellulos and lignin. The fermentable sugars in lignocellulose are derived from cellulose and hemicellulose (mainly glucose and xylose), but they are within an intricate structure that is recalcitrant to deconstruction and require a pretreatment (including detoxification and delignification). Indeed, pretreatment is the single most expensive element of the bioethanol process, representing about one-third of the overall processing cost. This operation aim is to remove lignin, hydrolyze hemicelluloses and make cellulose more accessible for enzymes allowing the production of fermentable sugars (glucose) in a further enzymatic hydrolysis stage. In the downstream microbial fermentation, the sugars extracted from celluloses and hemicelluloses are converted to ethanol. This work, unlike previous approaches addresses the environmental and economic impact of the pretreatment operations, including detoxification and delignification, in the biochemical production of ethanol from lignocellulosic biomass. Kinetic models are used to represent the pretreatment operations that predic the behavior and account for the main process variables that affect the entire process. These models are dynamic and include discrete decisions in the process design elements. The models have been implemented in the Jacaranda system for process design and optimisation. Results show the effect of decisions made in the pretreatment operations design on the whole process for the production of ethanol.

[660]

Model-based prediction and experimental validation of soap emulsions viscosities

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Soap is a very common end-consumer product which is used worldwide, with ten billion pounds produced per year. In Mexico, for example, the annual soap production industry is valuated 200 million dollars, making the soap production profitable. During the continuous saponification process, the emulsion viscosity is an essential variable which influences the conversion due to mass transfer limitations. Viscosity also impacts the operation of the downstream processing steps, such as the extrusion and the soap compression, to achieve the final product quality. Laundry soap emulsion viscosity prediction is complex due to the heterogeneous and variable composition: moisture, free sodium hydroxide, sodium chloride, sodium sulfate and fatty acids concentrations. Therefore, in this contribution the objective is to obtain a mathematical model via response surface methodology, to predict the emulsion viscosity for the system under study, which is the production of laundry soap in a facility located in Mexico: Jabonera Potosina S.A. de C.V. The methodology to develop such a model is the following: 1. Definition of the response property (viscosity). 2. Analysis of the variables that influence the viscosity: compounds concentrations, fat saponification value (FSV) and fatty acid value (FAV). 3. Determination of the level effects of the variables. 4. Create a response surface via a central composite design. 5. Performance of the experiments. 6. Analysis of the results 7.Model derivation. The obtained equation relates all the variables mentioned previously with the emulsion viscosity, and this will be useful to identify the operational adjustments in the process in different scenarios, such as the change of product from laundry soap to toilet soap.

[664]

A Novel Quantisation-based Integration Method for ODEs

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Quantised State Simulation (QSS) represents a paradigm shift in the numerical integration of ordinary differential equations (ODE's). Traditional numerical integration is based on the discretisation of time, which is treated as the free variable of the system. QSS mirrors this approach by discretising the state variables in such a way that variables are advanced one at a time towards the new value, the system dynamics dictate. Time in this scheme is computed a posteriori from the event that changed a state variable. The advantages of this approach are numerous as outlined in our work, particularly one can class them as: (i) effective decoupling of time scales of the system, (ii) direct and natural handling of discrete events in hybrid systems (no matter how frequent they are, the efficiency of the method remains effectively unperturbed), (iii) ease of extending the idea to handle stiff systems, (iv) efficient parallel schemes for the evaluation of parametric sensitivities, and (v) efficient schemes for the evaluation of ODE right hand sides exploiting Jacobian structures and the updating of the state vector one variable at a time. The latter can even be applied to densely coupled systems and does not depend on the sparsity of the system Jacobian. All these attributes have been researched in this work and extended beyond the current state of the art in QSS methods, offering a true alternative to the solution of hard dynamic simulation problems with high performance computing implementations in mind. Moreover, QSS bears great similarity in the "one variable at a time" approach as Stochastic Simulation does for the solution of ODE's but there the similarity ends: stochastic simulation approaches cannot handle with ease neither the parametric sensitivity issue nor the discrete events situation, while the QSS methods are inherently designed to handle these applications. While Stochastic Simulation is an effective way to simulate some classes of dynamic systems (that do not have frequent discrete events), they cannot generate stable and accurate gradients. That is imperative in parameter estimation studies (e.g. in combustion kinetics) as well as embedding the dynamic simulation model within an optimisation/design framework. As is shown in this work, these aspects are completely resolved with our proposed QSS approach, which in effect begins to emerge as a next-generation methodology extending dynamic simulation in a highly efficient and versatile way. Relevant applications will demonstrate the potential of the proposed approach.

[665]

A Novel Rigorous Mathematical Programming Approach to Construct Phenomenological Models

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The automation of the construction of physical laws from raw experimental or measurement data poses a great challenge in modern modelling technologies and to this date remains an open question. This work presents a novel generalised Mathematical Programming approach establishing a rigorous theoretical formulation that can capture any analytical function form in an iterative way and prove its adequacy in correlating data within measurement error tolerances and information theoretic measures. Unlike other approaches, our proposal is based on the use of generic representation of analytical functions as binary evaluation trees (Directed Acyclic Graph, DAG, representation form), which is the property they have and are defined by. The trees are constructed in such a way that their nodes are comprised of a linear combination of basic atomic functions, either arithmetic or unary, which are weighted by binary decision variables. Allowing only one such variable to attain the value of one, this forces the construction of a standard representation of any analytical function. It is theoretically demonstrated that as the tree expands, it is possible to encapsulate any analytical form a noiseless function may have, and given enough measurements to establish a unique fitting. For noisy data, as for example with measurements from experiments, suitable tolerance constraints can be included to ensure adequacy and reliability of the models extracted. The approach is generalised to capture the cases of dynamic models, e.g. models described by ODE right hand sides, as well as models that are described as series summations of terms. The premise to guarantee the solutions obtained is that deterministic global optimisation methods are used, otherwise with local optimisation techniques it is only possible to guarantee a sufficiently good fitting but not the absolutely best functional structure corresponding to the given data. To ensure further that the model is not overfitted, it is possible to include special zero-norm constraints that bound the number of nonzero parameters used in the derived models. The applications of this approach are envisaged to have significant impact in many diverse areas of interest: aside from physicochemical and biological systems, where for example one would be seeking to discover new interactions as well as their kinetic functional forms, it is possible to use this methodology in systems whose nature is not mechanistic, such as social systems, and offer quantification via novel model construction. We believe that our approach to construct phenomenological models, even for partially defined or understood systems, will lead to a significant advancement both in modelling approaches as well as revealing interactions that otherwise could not be discovered by heuristic trial-and-error, or mere observation of these systems. Relevant applications will demonstrate the potential of the proposed approach.

[685]

Modeling and Parameter Estimation of Enzymatic Biodiesel Synthesis

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The current work addresses to the modeling and parameter estimation of the biodiesel synthesis using supported lipases as catalysts. A kinetic reaction model was proposed in order to describe the enzymatic (trans)esterification reaction of vegetable oils and the set of kinetic parameters were numerically estimated with the direct search Complex and the Particle Swarm Optimization (PSO) algorithms. The proposed model and the parameter estimation strategy were evaluated, leading to a very suitable prediction of the process data. When the stochastic optimization procedures are compared, the direct search Complex algorithm is more efficient in terms of computation speed. In spite of this, both the Complex and the Swarm algorithms essentially conducted to the same kinetic parameter values. In summary, the general proposed model is able to predict very well the reaction behavior of all species into the reaction medium [triglyceride (TG), diglyceride (DG), monoglyceride (MG), glycerol (GL), alcohol (ROH), free fatty acid (FFA) and biodiesel (BD)]. Based on the algebraic-differential model performance, the proposed strategy can be successfully used to describe and optimize the biodiesel production through enzymatic reactions performed in batch and semibatch operating mode.

[692]

Analysis of two alternatives to produce Ethylene from Shale Gas

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In recent years, discoveries of shale gas have caused a decrease in the price of natural gas, which has opened a window of opportunities for the use natural gas not only as a source of energy but also as a feedstock for petrochemical processes. One such option is its use to produce ethylene, one of the main building blocks for many products such as plastics, resins and fibers. Although ethylene is produced from thermal cracking of ethane and propane from natural gas, alternative processes have been gaining increasing attention. These methods include the Oxidative Coupling of Methane (OCM) and the Methanol to Olefins (MTO) process; in both of them methane is used as a process feedstock. The OCM is a direct-conversion process in which methane is converted to ethylene using a catalytic reactor. The MTO is a process with several steps where methane has to be converted to syngas by a reforming stage, and then a catalytic reactor is used to produce methanol. The product, crude methanol, is finally converted to ethylene.

In this work an analysis of the production of ethylene from shale gas is reported. The analysis includes the assessment of economic, energy and environmental aspects. Process simulations using ASPEN Plus® were used for the technical analysis of the alternatives. The economic analysis includes the assessment of how changes in the prices of shale gas and ethylene affect the profitability of the processes. Based on pinch principles, energy conservation opportunities for each process are identified via targets for minimum energy consumption. Finally, the environmental analysis is based on the estimation of CO2 emissions for the two processes. The results show that the MTO process is more energy intensive, which affects its economic performance. Overall, the compromise among economics, environmental and energy implications for these production alternatives is reported.

[695]

A Crude Oil Econometric Model for PSE applications

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Crude oil quotations play a central role in the definition of prices of distilled products and derivatives. Manca (2013) showed how crude oil economics influences at a great extent also the quotations of commodities and utilities. Additionally, Mazzetto et al. (2013) used crude oil as the reference component for econometric models of bioprocesses and showed a functional dependency of both raw biomaterials and final bioproducts from the crude oil market.

The paper presents a number of econometric models proposed in the literature and compares their features with a new model specifically designed to be flexible and tunable enough to cover the specifications of both Conceptual Design and Supply Chain in terms of economic assessment over different time horizons. Indeed, these econometric models can be used to forecast the price of crude oil over short-, medium-, and long-term horizons, which are the time intervals intrinsic to PSE problems such as the scheduling and planning of supply chains, and the conceptual design of chemical plants. Once the crude oil econometric model is available, it can be used to model the operative expenses of chemical processes in terms of price/cost of raw materials, (by)products, and utilities. This point allows addressing issues such as market uncertainty, volatility of quotations, and price/cost fluctuations.

In addition, the paper discusses also the geographical localization of crude oil quotations that since 2011 have shown a division of Brent and WTI markets. This calls for a customization of parameters in econometric models according to the geographical region of influence where the economic assessment of either dynamic conceptual design or dynamic supply chain problems is carried out.

Finally, the manuscript discusses the time limit of the proposed econometric model and suggests the periodicity that should be applied in updating its parameters to produce reliable and consistent economic assessments of PSE applications.

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[711]

Simulation study of temperature distribution in the thermal drying oven for a lacquer coating process

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In a canning process, steel sheets must be coated by food-grade lacquer to prevent the corrison resistance caused by chemical reaction between products and containers. A lacquer coating process is divided into three main steps: coating, drying, and curing. In th drying step, lacquer flim on the coated steel sheet is removed. After that, in the curing step, chemical bonds between lacquer and surface of the steel sheet take place in the fashion of thermal curing. These steps are operated in the thermal drying oven. In the oven, a blower which normally operated under constant rotating speed delivers evaporated solvent or exhaust gas to be eliminated by incineration. In spite of unloading, the blower still drives to remove the exhaust gas leading to heat loss, the decrease in the oven's temperature, and insufficient consumption in electricity and fuel. Conseuently, an inverter, which can save electricity cost and increase thermal performance, has been implemented to control the operation of the blower by adjusting the rotating speed corresponding to a desired loading condition. In this work, temperature distribution of gas mixture between air and solvent in the thermal drying oven has been studied. Three dimensional heat transfer model with non-isothermal flow have been developed and validated by real data. Comparison of the temperature distribution between the conventional system and the new system with the inverter has been made. The simulation result showed that the system with the inverter can reduce the peak temperature in the oven leading to the energy saving of more than 15%.

[730]

Simulation and Optimal selection of distillation schemes for separating ternary mixtures

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Distillation is the mostly widely used industrial separation technique, but, at the same time, is the biggest energy consumer in process industries. For separation of a multicomponent mixture by distillation, there exist enormous possible flow sheet structures with different energy integration and/or thermal coupling configurations that can feasibly fulfill the task but may cost differently. How to find effectively the one that has the lowest energy consumption or lowest total annual cost (TAC) constitutes a veritable problem of Process Systems Engineering. However, it can be demonstrated that selecting an optimal distillation scheme among all the candidate configurations exhibits much more complications than that could usually be expected.

In the present contribution, rigorous simulations have been carried out for the separations of ternary mixtures by different distillation schemes. For any given ternary mixture of a given feed composition, simple distillation sequences with and without energy-integrations, side-rectifier and side-stripper (partially thermally coupled schemes) and dividing wall column (DWC, fully thermally coupled scheme) are optimized via the rigorous simulation. Then all the candidates are compared based on TAC as the criterion and the best one is selected. Six different ternary mixtures of different ease of separation index (ESI, defined as the ratio of the relative volatility between components A and B to that between components B and C, with A, B and C ranked in terms of their volatilities) with various compositions are used in the investigation. The triangle maps of the feed compositions are explored such that for a ternary mixture, any point on the map is used as the feed composition and the best distillation scheme is selected. Then, based on the best selections for sufficient number of points, the triangle map is divided into different areas, in each of which the best distillation scheme is identical.

In such a way, boundaries of different distillation schemes on the corresponding triangle maps are obtained for different values of ESI. The results demonstrated that a traditional distillation sequence with energy-integration or thermal coupling may win over the DWC in many cases, and the subjective use of a DWC may lead to energy loss in those cases. Using the results, we finally propose several simple heuristics for the selection of optimal distillation schemes for the design.

Maria-Ona Bertran, Thomas Bisgaard and Rebecca Frauzem (Eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. 31 May - 4 June 2015, Copenhagen, Denmark

[736]

A neg-entropy interpretation in a biochemical process: an attractor model with cell duplication

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With the development of biotechnology, biochemical engineering has received unprecedented attention as a new means to provide human society with the material and energy they need, and to a large extent, biotechnology challenges the traditional physical or chemical approach for mass and energy extraction on social, environmental, and economic perspective. While tremendous work has been done on microbial metabolic pathway identification and reformation, few publications are targeted on mass flow and energy transformation from a process point of view. Microbial growth is normally operated far from equilibrium, and it is a dissipative structure system. With neg-entropy constantly flowing into it, microbial system evolves and becomes more organized. In a biochemical process, microbial can be viewed as a mass attractor, where the nutrient is aggregated; it also can be viewed as an energy attractor, to which energy quality level is upgraded. In this research, a case study of microbial fermentation of wastewater containing starch for biodiesel production is implemented. An attractor model with cell duplication is proposed to quantify nutrient intake rate in Rhodotorula glutinis. With this model, the apparent nutrient concentration of the attractor, which represents the broth/microbial interface mass concentration, is evaluated with experimental data, and it is the lower limit of fermentation broth. The concentration deviation acts as the driving force for mass aggregation to the attractor. The entropy change of the broth is calculated, which is difficult to quantify without the attractor model since the fermentation broth is an open system. The entropy flux to the attractor represents the effect of the attractor in upgrading energy quality level, and it can be used as an evaluation index for different biochemical processes. Both the apparent mass concentration and the neg-entropy flux of the attractor are well defined and have physical explanation; and they can be used as a guide to real time practice.

[756]

Integration and optimization of an air separation unit (ASU) in an IGCC plant

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An integrated gasification combined cycle (IGCC) is a promising green technology applied for thermal power plants. It offers an efficient way to generate electricity from coal, biomass or any other suitable solid or liquid fuels with lower impact to the environment. The biggest challenge of making IGCC to become a viable technology is its high energy production cost. This creates a barrier for this green technology to enter into the stage of a highly competitive electricity market. An IGCC plant is a complex process system that involves processing units operated in very extreme conditions. Proper material and energy integration may provide a hope for cost reduction. In this paper, a mathematical model of an IGCC plant was built that includes a gasification unit, an air separation unit (ASU) and a combined cycle unit. A modified Gibbs free energy model is used for predicting the composition of the syngas taking into account material and energy balances. The proposed gasification model results in syngas composition similar to the experimental data provided in literature. The modified gasification model is combined with the rigorous distillation model in ASU and two different pressure-level turbines in combined cycle unit. Although individual processing unit optimization plays a significant role in enhancing the plant performance, an optimal integration among the three units still has significant potential to improve the efficiency, availability, and operability of a coal-fed IGCC power plant. The proposed mathematical model allows material and energy integration to be performed within and among different processing units while optimizing the IGCC plant as a whole. An optimization procedure is proposed that simultaneously optimizes the integrated plant. Different material and energy integration schemes were studied with respect to the total cost and the overall thermal efficiency of the integrated plant. Pinch analysis is applied to show the effectiveness of different design options and to provide guidance for further improvements.

[757]

Mathematical Modeling of an Industrial Delayed Coking Unit

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This paper describes the mathematical modeling of the physical-chemical phenomena in the coking furnace and the in coke drum in a steady-state delayed coking unit. Delayed Coking is a thermal conversion process, known in the petroleum industry as "bottom of the barrel". The proposed model is based in lumped kinetic scheme and vapor-liquid equilibrium conditions. For the development of rigorous models including detailed chemical reaction kinetics, feedstock and products composition, and so on, molecular structure are required. For this work, molecular characterization of crude oil and heavy fractions was carried out mainly by MALDI TOF mass spectrometry. Then, the model provides detailed understanding of the coking process and the effect of the feedstock physical-chemical properties on yields and quality parameters of the products, especially the petroleum coke produced. Mathematical algorithm has been developed to determine the kinetic parameters and simulate the process. Experimental data and operating conditions from an industrial delayed coking unit are being used. The expected result is a good prediction capability of the proposed mathematical model and consequently an accurate representation of the industrial unit. Process simulation based on the rigorous model will help process engineers in the petroleum industry with some insights on coking furnace and coke drum operation. Moreover, the developed model will be used for monitoring the industrial process and implementing real time optimization (RTO). Meanwhile, the acquired knowledge obtained during the model development has improved the quality of green coke produced and the operational procedures of industrial plant.

[762]

Post-combustion CO2 capture with sulfolane based activated alkanolamine solvent

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Carbon dioxide capture from the flue gas streams of fossil fuel based power plants and its sequestration (CCS) has received global attention due to the environmental need to substantially reduce the emission of CO2 to the atmosphere to mitigate the global warming problem. For post-combustion CO2 capture (PCC), regenerative chemical absorption is still the process of choice for the power plants [1]. At present the major focus of global CCS research as well as this study is on the development of more efficient solvents with higher CO2 capacity, higher rate of absorption, lower regeneration energy in order to reduce the prohibitive cost of capture. In this work n-methyldiethanolamine (MDEA), a non-carbamate former tertiary alkanolamine is chosen as the base amine. Piperazine (PZ), a high reaction rate cyclic diamine, is used as a rate activator along with aqueous MDEA. Besides the PZ-activated MDEA solvent, the hybrid solvents are prepared by adding a physical solvent, sulfolane (tetrahydrothiophenedioxide), in which CO2 has high solubility, into the activated solvents.

Vapor-liquid equilibrium (VLE) of CO2 in PZ-activated MDEA and in the hybrid solvents have been measured over the temperature range of 313-333 K with a high pressure stainless steel stirred equilibrium cell. A detailed description of the experimental set up is presented by Dash et al. [2]. ENRTL theory has been used to model the VLE of (MDEA+PZ+H2O+CO2) and (MDEA+PZ+Sulfolane+H2O+CO2). There is good agreement between the experimental VLE results and model results with an AAD of less than 7.6%.

Process simulation software Aspen Plus (V 7.1) [3] has been used for estimating the percentage CO2 capture from coal based flue gas by absorption at steady state conditions using aqueous MDEA, PZ activated aqueous MDEA and the hybrid solvent. The Aspen absorber-stripper flow sheet model has been used. The absorber column has been modeled using RedFrac model of Aspen Plus. The simulation work has been carried out to study the effect of different parameters e.g., L/G ratio, absorber pressure, packing height and amine concentration on %CO2 capture.

From the simulation study it is observed that the %CO2 removal is higher with all hybrid solvent formulations compared to that with PZ activated aqueous MDEA solvents. At an L/G ratio of 3 the hybrid solvent (42 mass% MDEA+8 mass% PZ+10 mass% sulfolane + 40 mass% H2O) achieved 85% CO2 capture at 40oC. All hybrid solvents have been found to have about 35-40% higher solvent capacity compared to that of the corresponding activated amine solvents.

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[769]

Modeling and Sensitivity analysis of a medium-temperature gas cleaning process of biogenous synthesis gas

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Biomass gasification is a promising option for the production of electricity, fuels and other chemical components. Usually the product gas contains unacceptable amounts of tar, causing operational problems in the downstream processes due to possible tar condensation.

A novel and innovative catalytic gas cleaning process, operating in a considerably lower temperature range than Catalytic Hot Gas Cleaning Methods was developed in the course of a previous project. In the medium-temperature gas cleaning process the synthesis gas is cooled to 300°C after the gasifier. After a shifting number of desulfurization steps, the product gas passes a catalytic reactor. In this step Nickel is used to catalyze the methanation-reaction as well as the steam reforming of hydrocarbons. The exothermic methanation-reaction leads to a temperature rise in the reactor of up to 600 °C.

The focus of this work lies in the process design and the simulation of a small-scale production of Raw-SNG (Substitute Natural Gas). Thermodynamic models for the individual gas cleaning steps are developed and implemented into an already existing model library of the commercial simulation software IPSEpro. Mathematical models for the different desulfurization steps, the scrubbing as well as the tar removal and methanation of the biogenous synthesis gas are provided by applying mass and energy balances and reaction kinetics and chemical equilibrium equations. To evaluate the impact of impurities and the operational costs, catalytic deactivation and consumption of consumables are considered in the models.

Based on an allothermal gasifier, the so-called heat pipe reformer, the whole process is integrated into the simulation software using these mathematical models. To identify energy savings and increase the efficiency of the overall system, the optimized thermal integration of the single process steps is determined.

Additionally, a sensitivity analysis is performed to show the influence of different operating parameters, e.g. process pressure, excess steam ratio or the product gas temperature at the inlet of the catalytic stage. Their effects on the overall process efficiencies as well as on important process factors are evaluated and discussed in this paper.

[788]

Exergy Analysis of Monoethylene Glycol (MEG) Recovery Systems

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Hydrates are ice-like crystalline compounds comprised of water and natural gas, and its formation in natural gas pipelines can lead to several problems in Oil and Gas Industry, such as pipeline blockage, leading to serious operational and safety problems. To avoid these undesirable problems, the injection of hydrate inhibitors in wellheads has been widely employed. Among several options for thermodynamic hydrate inhibitors, in the present work Monoethylene Glycol (MEG) was chosen due to presenting a series of advantages when compared to other thermodynamic and non-thermodynamic inhibitors.

As MEG can be reused, its re-concentration and salt removal are necessary before recirculation through subsea pipelines, in order to avoid salts accumulation and saturation, which entails scaling and other concerns. MEG Recovery processes can be divided into three types: Traditional, Full-Stream and Slip-Stream Processes. For evaluating these processes, Aspen HYSYS Software was used for simulation.

A better understanding is attained when a more complete thermodynamic view is taken. In this sense, a comprehensive analysis of a thermodynamic system includes both energy and exergy analyses in order to obtain a more complete picture of system behavior.

Exergy is the maximum amount of work obtainable when a system is brought into equilibrium from its initial state to the environmental state. In this regard, Exergy is a property that depends on the state of both the system and environment. Unlike energy, exergy is consumed or destroyed due to irreversibilities in any real process and thus provides deeper insight into process analysis.

It was developed a methodology of exergy analysis based on the First and Second Laws of Thermodynamics. This exergy analysis intends to evaluate the thermodynamic efficiency of the processes by estimating the associated percentage of destroyed exergy.

Further, for the reference environmental state, two approaches were used: one using the reference environment as atmospheric air only, and the other one using the reference environment as air saturated with water in equilibrium with MEG infinitely diluted in water.

Those 2 approaches led to different results, but, in both cases, the Full Stream Process had the highest energy consumption, while the Traditional Process had the lowest energy consumption, with Slip Stream Process occupying an intermediate position. Regarding the exergy efficiencies, the Traditional Process was the most efficient, whereas the Full Stream Process was the less efficient and, again, Slip Stream Process occupied an intermediate position. The results are as expected, since the Traditional Process is the simplest and therefore leads to lower energy consumption and lower exergy destruction. Full Stream Process, in comparison with Slip Stream Process, treats the largest amount of material flow and therefore has a higher energy consumption and higher exergy destruction.

[822]

Production of Biodiesel via Enzymatic Palm Oil Ethanolysis: Kinetic Study

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Biodiesel is an alternative fuel that has become attractive due to its environmental benefits compared to conventional diesel. This biofuel can be obtained through different routes, being the transesterification of edible/non-edible oils or animal fat with an alcohol, the most used. Methanol is the predominantly alcohol used for this reaction, although ethanol produced from sugarcane represents a good alternative since is non-toxic and is widely available in Brazil.

Despite the alkaline catalyst be the most frequently employed for the synthesis of biodiesel, the difficulties associated with the glycerol recovery, catalyst removal and the purification steps motivate several researches related to the enzymatic transesterification since through this route such problems are non-existent.

Over the years an initial reaction rate based on the Ping Pong Bi Bi enzyme mechanism has been adopted to represent the kinetics of the enzymatic transesterification in several references in the open literature. However, in this work, a two parameters model taking into account the inhibitory effects due to the concentration of both product species was proposed and the experimental oil conversion data were fitted to the model.

The kinetic study of the palm oil ethanolysis reaction catalyzed by immobilized lipase Novozyme 435 (from Candida antarctica) has been made in a temperature of 42°C and 4% of catalyst based on reactants mass at atmospheric pressure. A maximum conversion of 70% of oil was obtained after 6 hours of reaction.

The model was successful in predicting the experimental data behavior (mean absolute deviation <2%) with the reactor operating in a batch model and the kinetic constants have been determined for the model proposed within the experimental condition studied. The estimated standard errors in both parameters were small compared to with their values, ratifying with the excellent fit of the rate equation proposed.

[827]

Integration of retrofitted coal-fired power plant with CCS: Power derate minimization

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Carbon dioxide (CO2) capture and storage (CCS) have attracted worldwide attention as a near-term technology to decelerate global warming. Especially, post-combustion CO2 capture has an economic advantage by utilizing existing coal-fired power plants. Furthermore, aqueous monoethanolamine (MEA) scrubbing is the most widely implicated method among other capture technologies. However, the necessity of heat and energy requirement for the solvent regeneration and CO2 compression cause 15-30% decrease in net power output, which is power derate, by steam extraction and energy consumption. This power derate is a major obstacle to implementing CCS into power generation plants. To reduce power derate, much research has focused on not only developing new configuration of the individual process but also integrating the processes with existing power plants. Unfortunately, none of previous research conducted power derate minimization through multivariable optimization even though power derate of the integrated process is affected by a lot of interrelated variables. In this study, simulation-based multivariable optimization of coal-fired power plants integrated with CCS process is performed in order to minimize the power derate. This work undertakes the simulation of post-combustion CO2 capture with aqueous monoethanolamine (MEA) scrubbing and CO2 liquefaction process integrated with a 550 MWe supercritical coal-fired power plant using Aspen Plus V7.3. Liquid to gas ratio and stripper operating pressure of CO2 capture process and compression ratio of CO2 liquefaction process are chosen as manipulated variables based on the variable evaluation. Steam extracted from IP-LP crossover pipe and the first LP turbine are considered as possible heat sources respectively. As a result, power derate is minimized from 32.6% to 17.3% when operating at optimum conditions.

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[828]

CUDA-optimized cellular automata for diffusion limited processes

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A lot of chemical technology processes in porous media are limited mainly by diffusion mass transfer. Adsorption, drying and chromatography are good examples of such processes. After certain time the process depends only by molecular diffusion in disordered porous media and energy interactions between moving particles in mobile phase and stationary solid body. Modelling of this processes demand for taking into account transport properties including tortuosity, permeability and local characteristics of the internal structure. Especially all those properties are hard to estimate for high porous disordered media.

In this work aerogels were chosen for modelling. Aerogels — are very perspective materials with unique properties such as low density, high internal surface area, low thermal an electric conductivity and with diameter of pores in only about few nanometers. The stochastic model of aerogel structure was developed for further simulations.

Cellular automata (CA) approach was used for molecular diffusion modelling. The transition rules allows to take into account main mass transfer processes that drive system to thermodynamic equilibrium: diffusion, adsorption/desorption and directed flow. CA simulations even in small scales show good similarity with real world systems.

Use of parallel computing (process level parallelism and GPU-based CUDA technology) in all stages gave from 5x to 100x speed up in comparison with standard sequential realisation.

[842]

Effect of ship motion on amine absorber with structured-packing for CO2 removal from natural gas: An approach based on porous medium model

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Acid gases (H2S and CO2) must be removed from the crude natural gas. The process performance may be deteriorated because of ship movement on FPSO (Floating production, storage and offloading). This research aims to investigate the effects of ship motion on acid gas removal performance in the amine absorber with Mellapak 250.X structured packing.

A simple cylindrical column (packed zone: 0.1m diameter × 0.98m high) was used as the domain for the calculations. A porous media CFD (computational fluid dynamics) model was used in the framework of Eulerian two-fluid flows with user-defined functions (UDF) taking into account liquid dispersion and mass transfer in the packed zone. The effective interfacial area, mal-distribution factor and CO2 concentration profiles were compared for two cases of vertical standing and ship motion. The numerical result shows that the ship motion has the negative effects on the absorption efficiency.

[852]

Model-based analysis and efficient operation of a glucose isomerization reactor plant using a Systematic Integrated Framework

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The importance of the application and the use of model-based methods in the analysis and the operation of chemical/biochemical/pharmaceutical processes has been highlighted by many authors [1, 2]. The development of mathematical models requires a high level of understanding and a detailed analysis of the phenomena which take place in the different systems [1, 2]. Moreover, the use of systematic approaches for the development and improvement of mathematical models is also of great importance, especially because the re-use of the mathematical models becomes easier and more efficient [1].

In this work, an integrated systematic framework is used, with the objective to assist the multi-purpose manufacturing industry to systematically solve the multiple complex problems in order to move from batch to continuous manufacturing by using systematic model-based methods. This framework, consists of four different parts: The first part, "Part A: Reaction Mechanism Identification", identifies the reactions which take place in the system. The second part is "Part B: Reaction Analysis", where all the reactions are analyzed with respect to the involved compounds, the reaction conditions, the reaction kinetics, the effect of different reaction variables and the reactor design. The third part, is "Part C: Process Synthesis and Design" where the process is synthesized and designed based on the driving force principles. The final part is "Part D: Simulation, Operation, Optimization and Control" where the developed process is simulated, evaluated with respect to economic and sustainability metrics, and finally optimized and controlled.

The objective of this work is to use the necessary parts of the integrated systematic methodology on an industrial case study of the glucose isomerization (GI) reactor part of a corn refinery. A typical plant consists of a number of parallel GI columns with different specifications (column height, operation temperature and column lifetime). Therefore, the purpose of this study is to develop a reactor model which includes the kinetic model as a function of temperature, the energy balances and the enzyme activity decay as a function of the temperature including the diffusion term. The developed mathematical model is intended to be used for the simulation of the reactor plant and validated against experimental data for different reactor conditions such as temperature and flow rate. The outcome of this case study is to improve the operation of a typical GI reactor plant in order to improve the productivity of the plant. Also, based on this simulation model, a planning and scheduling problem is defined and solved for further improvement of the plant operation. Finally, the developed model needs to have the flexibility to be adapted fast such that it can be used to simulate and improve operation of similar processes.

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[863]

An automatic generation of reactor models and simulation in an object oriented fashion

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Industrial reactors manifest in a variety of different sizes, flow configurations and designs. This diversity is due to differences in the kinetics, stoichiometry of reactions, hydrodynamics, reactor shape and size, thermodynamics and heat transfer conditions. The modelling and simulation of industrial scale reactors requires a detailed understanding of these phenomena along with the mathematical implementation in computer system. The research work reported in this paper extends the object oriented representation of this diversity presented by Moharir et al. (2001) and Mandaliya et al. (2012).

Generic classes for reactor kinetics, stoichiometry of reaction, hydrodynamics, reactor shape, thermodynamics and heat transfer conditions were defined. The general mass, momentum and energy conservation equations in dynamic forms were integrated over the user defined shape of reactor, boundary conditions for heat and mass transfer, thereby achieving automatic generation of reactor models in C++ string format. These generic classes were instantiated at the run time based on user description to give a specific instance of the reactor as a C++ object. A solver class object intuitively selects various solution methods, viz. finite difference methods, method of lines, and Green's function method for the efficient solution of the resulting reactor models object.

A numerical analysis is presented in this paper using the various solution methodologies, i.e. comparison of analytical solution with the numerical solution. The proposed framework has been tested for (i) Non-ideal reactor, (ii) Industrial scale varying area reactor, and (iii) Annular reactor configuration. It has been shown that the above cases can be modelled from the same generic class depending on the user description. A comparison of solution strategies using Finite Difference Methods is presented. The framework is capable of creating transient 3-Dimensional conservation equations, though solution/results presented here have been restricted to steady state 2-Dimensional homogeneous and pseudo-homogeneous reactor models.

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[864]

Fluidized Bed Reactor for Solar-grade Polysilicon Production: CFD and silicon growth simulation study based on time scale analysis

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Photovoltaic industry is expected to grow faster in the second half of the present decade, primary due to environmental reasons and chase for alternative energy source. Polysilicon, in the form of granules or multi-crystals, is the primary feedstock in modern photovoltaic industry. The conventional commercial technology for silicon (Si) production process, Siemens Reactor is said to be highly stable, but has certain darwbacks in terms of high energy consumption and low yield due the need to operate in batch mode rather than in a continuous mode. Due to this, in today's commercial environment, a fluidized bed reactor (FBR) has become an attractive technology, as it can offer competitive advantage over Siemens process, in terms of energy saving, low production cost, higher yield and easier product handling. However, FBR technology for polysilicon production also comes with its own inherent chanllenges--the challenge to achieve a stable operation. Hence, a number of researchers have already studied FBR technology for polisilicon production through numerical approach to understand the emergent behavior that may arise from a typical operation of an FBR technology. But a comprehensive model simulation that explain the inter-linkage between the hydrodynamic behavior and particle growth is still missing. In our study, we try to show the temporal change in hydrodynamic behavior as the silicon particle grows. For this purpose, we first carried out time scale analysis of hydrodynamics, reactions and particle growth. Based on the time scale analysis, simulation strategy for Computational fluid dynamics(CFD) module and silicon growth and particle dynamics module was decided. CFD module considers the hydrodynamics inside the reactor arising from gas-solid interactions. Eulerian-Eulerian two fluid model of ANSYS FLUENT with kinetic theory of granular flow for the solid phase and k-epsilon turbulence model for both the phases, was used to simulate the gas-solid flow. Silicon growth and particle dynamic module considers growth of siliocn seeds to full product size silicon granules.The simulation approach considering only the hydrodyanmic was first validated by carrying out simulation for a fludized bed system given in literature(Muthu and Nataranjan, 2008). FBR design of Jet Propulsion Laboratory(JPL) was used for the combined hydrodynamic and silicon grwoth simulation study. Experimental data in terms of mean diameter of product silicon from JPL was used to compare with the results from present simulation. The reactions in polysilicon formation process are driven by externally maintained high reactor temperature. The effect of reactor temperature on the hydrodynmic behavior and particle growth was also studied.

[868]

pyIDEAS: an open-source python package for model analysis

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Mathematical models are used in many scientific areas such as enzyme kinetics and process engineering. They can be used for process analysis and optimization. However, a model is always a simplified representation of the real process and predictions always come with uncertainty. Therefore, the model building process should be performed thoroughly addressing calibration and validation procedures. Specific modeling tools (e.g. sensitivity analysis, optimization algorithms, experimental design techniques,…) to derive additional information (e.g. importance of parameters, parameter estimate uncertainty,…) are at hand and available in existing software. First, implementing these algorithms is time-consuming and often suboptimal in efficiency. Second, existing software is in many cases closed-source and not flexible in use. In both cases this results in the unavailability of the programmed algorithms in the corresponding articles making use of them. Therefore it is hard to validate the published findings and in some cases even impossible to reproduce the presented results. To address this problem we need a certain critical mass of algorithms to perform model analyses which are available to the modeling community. To improve overall quality and reliability, such kind of code library should be open-source and well documented.

We hereby present pyIDEAS, an open-source Python package to thoroughly but swiftly analyze systems represented by a set of (possibly mixed) differential and algebraic equations. The pyIDEAS package allows performing a model analysis in a straightforward and fast way. Speed enhancements were mainly achieved by using optimized routines provided in the Numpy, Pandas or Sympy packages. Currently the package contains the following tools: solving differential algebraic equations, local sensitivity analysis, model calibration, Optimal Experimental Design (OED) for parameter estimation and parameter and model confidence calculations. pyIDEAS provides a well-structured and logic framework which allows non-programmers to perform a basic model analysis and more advanced users to extend or adapt current functionality to their own requirements. The pyIDEAS package will be presented by means of accessible examples. In the near future the package will be extended with identifiability analysis to get information whether a selected set of model parameters can be uniquely calibrated or not given a set of experimental data.

[874]

A numerical procedure for model identifiability analysis applied to enzyme kinetics

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The proper calibration of models describing enzyme kinetics can be quite challenging. In the literature, different procedures are available to calibrate these enzymatic models in an efficient way. However, in most cases the model structure is already decided on prior to the actual calibration exercise, thereby bypassing the challenging task of model structure determination and identification. Parameter identification problems can thus lead to ill-calibrated models with low predictive power and large model uncertainty.

Every calibration exercise should therefore be preceded by a proper model structure evaluation by assessing the local identifiability characteristics of the parameters. Moreover, such a procedure should be generic to make sure it can be applied independent from the structure of the model. We hereby apply a numerical identifiability approach which is based on the work of Walter and Pronzato (1997) and which can be easily set up for any type of model. The presented approach consists of four main steps: first, in silico data is generated by using a certain model structure and different parameter sets. Second, random noise is added to this artificial data; this procedure is repeated many times to ensure that, from a global point of view, noise can be regarded as random. In the third step it is tried to retrieve the original parameter set for each of the noise corrupted data by means of an optimization algorithm (local or global). The final step is to visualize the histograms of the different parameters retrieved from all the optimisations. In this way the uncertainty for each parameter, assuming a certain noise level, can be obtained in a quantitative way. When distributions are retrieved that are either uniform or shifted with respect to the parameter value used in step 1, a practical local identifiability issue is revealed. The technique was applied to the forward reaction rate of the enzyme kinetics proposed by Shin and Kim (1998). The practical identifiability analysis revealed that high values of the forward rate parameter Vf led to identifiability problems. These problems were even more pronounced at higher substrate concentrations, which illustrates the importance of a proper experimental design to avoid (practical) identifiability problems. By using the presented approach it is possible to detect potential identifiability problems and avoid pointless calibration (and experimental!) effort.

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[886]

Dynamic simulation of a batch aqueous two-phase extraction process for alpha-amylase

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The market for therapeutic proteins is currently increasing at a remarkable pace. In many cases, therapeutic proteins, such as monoclonal antibodies, must be administered in relatively large dosages. This large dosage requirement (> 100 mg dose-1) [1], coupled with the high demand for these drugs, has resulted in an increased pressure on pharmaceutical companies to deliver high quality drugs at sufficient quantities. As a result, there has been an increasing amount of research & development (R&D) aimed at improving upstream efficiency, which has resulted in increased cell titres during the cell culture/fermentation stage of protein production. To date, improvements in upstream technology have, however, not been matched by improvements in downstream technology. Consequently expensive chromatography columns must be scaled accordingly to cope with the increasing amounts of material generated, which is proving to be a process bottleneck due to the limitations in their capacity, but also their cost, and has highlighted the need for a re-evaluation of downstream separation methodologies.

Aqueous two-phase systems (ATPSs) are a promising downstream separation technology in the production of biopharmaceuticals. Understanding the fundamentals of protein separation is challenging due to the large experimental space that must be explored. To tackle this, experimental liquid-liquid equilibria and protein partitioning data is combined with a process model to explore the dynamic operation of a semi-batch aqueous two-phase extraction process for the separation of enzyme α-amylase in a PEG 4000–phosphate ATPS containing NaCl. The semi-batch system can be readily implemented into existing biopharmaceutical production processes. Interaction parameters for chemical potential equations are estimated from tie-line data. Running multiple extraction cycles, where the bottom phase is replaced with fresh phosphate rich, protein free material, increases the purity of α-amylase while reducing the yield. The influence of the phase ratio on α-amylase purity and yield is also investigated.

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[908]

Integrated Simulation Platform of Chemical Processes Based on Virtual Reality and Dynamic Model

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Due to the upcoming shortages of plant operators, more and more simulation platforms are widely developed for training. However, the conventional simulation environment is not intuitive for the beginners. In this study, a new integrated simulation platform based on virtual reality and dynamic model was proposed. Realistic 3D model of the chemical plant was developed which interacts with the dynamic model and the companied control system. Also the scene on site was integrated for monitoring the real process conditions. With the OPC interface, the dynamic model could run simultaneously with the actual plant. As a case study, the integrated simulation platform of ethylene process was illustrated. The simulation results showed that the integrated platform is more friendly and accurate to be used for training operators.

[912]

Application of PSE Methods and Tools in the Development Reliable Property Prediction Models for Lipids

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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. Since all property models require parameters estimated from measured related to property data, a collection of data is necessary before any property models can be developed, tested and applied. However, the measured data may be inconsistent and so a consistency check is necessary. In order to make the property models predictive, a scheme to extrapolate from the measured data is necessary. For this, the group-atom contribution method has been found to be suitable. For application in model-based design-analysis, etc., property models applicable for a wide range of chemicals and their mixtures for the needed properties. This requires a suit of models, their associated model parameters and information on their applicability. Another important issue is the uncertainty of the model predictions – they need to be quantified.

PSE methods and tools are ideally suited for the above mentioned tasks and they have been adopted to develop schemes for property data consistency tests, optimization based data regression to estimate the model parameters, knowledge representation and search engine for database development and use and finally, computer aided modelling tool to quickly and efficiently develop the necessary property prediction models. The presentation will highlight a specially developed property prediction tool for lipids with its built-in database, consistency check for measured data, parameter estimation feature and estimation of a large collection of pure component and mixture properties involving lipids. The tool also has a library of pure component and mixture property models such as the group-atom contribution based models for pure component properties, UNIFAC and PC-SAFT for prediction of phase equilibrium related properties of mixtures. The application of the developed properties models will be illustrated through case studies involving different lipid compound processing steps.

[920]

OsmoseLua - An integrated approach to Energy Systems Integration with LCIA and GIS

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In this paper, we present our recent work on the implementation of an Energy Systems Integration platform which allows modeling Energy systems sharing LCI (Lifecycle Inventory), LCIA (Lifecycle Impact Assessment) and GIS (Geographical Information Systems) data as accessible modeling parameters and variables.

Being based on our previous experience in methodologies and models of Energy System Integrations, we developed a new generation of a platform using a script language called Lua. The main motivation of choosing Lua was to radically improve the performance problem, which was the main drawback of our existing Matlab-based system, while proposing a more convenient way of describing the Modeling elements and their combination.

Second objective of our work was to integrate LCI and LCIA aspects as a generic part of the Energy systems modeling methodology. As for the LCIA, we have succeeded in integrating Ecoinvent3 LCIA analysis datasets as Energy modeling variables which are accessible during the optimization modeling. As far as LCI elements are concerned, we achieved in extracting generic LCI datasets corresponding to some selected Energy Modeling Element. Such a categorization is essential in order to give a certain level of reusability regarding LCI datasets which are in general huge in volume. Currently we are working on the process data mapping algorithm in order to find appropriately the UProcess' or EFlows' ID used in Ecoinvent3 databases.

Thirdly, by giving the possibility of importing GIS databases (in csv format as its first trial), some coordination data, such as longitude and latitude, can be directly included as Energy System elements' locational parameters. This possibility gives a great efficiency in modeling urban systems energy integration modeling, within which building's locations or heights play an important role of model constitution.

We could verify that such an approach can not only improve the simulation time performance but also provide a high level of modeling efficiency.

[921]

Incremental Kinetic Identification based on Experimental data From Steady-state Plug Flow Reactors

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The distributed reactors such as plug flow reactors, axial flow reactors are often used in chemical process industries. Thermal cracking, catalytic gas phase reactions etc., are some examples where these reactors are employed in industries. Plug flow reactors are often used to identify reaction kinetics for these reactions in the laboratory [1]. These experiments of kinetic identification are performed at steady-state operation of the reactors where the concentrations at the inlet and outlet of the reactor are often measured. Then, these data are analyzed using the simultaneous kinetic identification approach [2].

Recently, the incremental approaches have been proposed to identify reaction and mass-transfer rates based on experimental data from tank reactors [2]. The incremental approaches decompose task of identification into a sequence of subtask such as the identification of stoichiometry and rate expressions. Hence, the number of model candidates can be kept small in each subtask, and the information available from one task can be used in the subsequent steps. The incremental kinetic identification approaches can be classified as: (i) rate-based methods, and (ii) extent-based methods [3,4]. A comparison of these approaches has been given in [4]. The best of our knowledge, these approaches have not been developed to analyze experimental data from plug flow reactors.

In this work, we extend the incremental kinetic identification to analyze concentrations data from non-isothermal steady-state plug flow reactors (SPFR) with tubular geometry. A model of non-isothermal SPFRs consists of the material and energy balance equations of SPFR in form of a set of differential equations. Since SPFRs often are used for studying gas phase reactions, the pressure drop equation will also be included. Three scenarios of reaction operations and concentration measurements are distinguished: (S1) concentrations of species are measured along the length of reactors, (S2) concentrations of species in the outlet stream are measured for a given inlet concentration condition at various volumetric flowrates, (S3) concentrations of species in the outlet stream are measured for various inlet conditions. For Scenarios S1 and S2, it is shown that the extent-based incremental identification can be applied to concentration data. For Scenario S3, it is shown that the rate-based incremental identification can be applied to concentration data. All scenarios are corroborated with a simulated example of pyrolysis of dimethylformamide in a non-isothermal tubular reactor.

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[941]

Nonlinear fuzzy identification of batch polymerization processes

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First-principles-based modeling of polymer systems is usually complex and time-consuming, often leading to correlations of restricted range of applicability with unavailable parameters. Thus, the model-based optimal control of such processes is very tricky, especially when tracked batch reactors in which the systems move from one steady state to another or never reaches a steady state at all. Although classic modeling approaches have still been commonly used, new learning technologies in process engeneering that allow better, simpler, and more accurate behavior predictions have recently been introduced.

This paper describes the application of the fuzzy logic to model batch polymerization reactors. The proposed fuzzy methodology allows the formulation of a global nonlinear long-range prediction model from the conjunction of a number of local linear fuzzy dynamic models. Here, beyond building reliable fuzzy models, it is focused the selections of an appropriate model structure for a future design of advanced controllers. Such generated fuzzy output is fed back to the fuzzy structure to calculate the current output through one or more time delay units.

The production processes of Poly(Lactic Acid) (PLA) and nylon-6 were adopted for performance evaluation of proposed method. The reactions were carried out in a scale laboratory pilot-plant. A rigorous phenomenological model is available for such system. The mathematical model for the PLA process is solved by a Runge-Kutta type algorithm implemented in C++ programming language and, for the production of nylon-6, the equations system was implemented in Aspen Plus process simulator. So, the two resulting computational programs were experimentally validated and they are considered as virtual plants for obtaining of identification dynamic data. Additionally, data sets from experimental measurements were used. Then, appropriate techniques for fuzzy models indentification procedure were used and the formulations were built in both Fortran 90 and Matlab platforms.

Satisfactory results were achieved from the pilot-plant point of view. This supposes that the proposed method can be useful to obtain appropriate representations of systems of difficult modeling and it can be applied in several ways, as on the tracking of processes well as on optimization techniques and advanced control.

[960]

Modeling dissolution of solids based on cellular automata with changing sizes of cells

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To date, there are several models describing the process of dissolution of solids. The most widely used models based on cellular automata. All the previously known models of dissolution based on cellular automata cells have a fixed size, which imposes certain restrictions on the model. Proposed model for the dissolution of solids based on cellular automata with changing sizes of cells avoids the disadvantages of previous models.

The calculation of the dissolution process is performed as follows. As input parameters is given linear size of the field - N cells, and the maximum content of each substance in the volume of cell. Changing the amount of substance in each cell in time proportional to the diffusion coefficient multiplied by the surface of contact area of the interacting cells and the difference in the contents of substances in them.

In the process of dissolution out of cells with the solid substance goes into the cells with a liquid, consequently, the amount of the substance in the cells changes. On this basis, we can assume that the distance between the cells changes. In all pairs of cells liquid - solid their boundaries are shifted toward cells with the solid. Linked matrix enables to resize cells, or even to remove the cells (at the solid fully dissolved). Linked matrix contains a distance between eight neighboring cells.

This model based on cellular automata with changing size of the cells has several advantages:

- makes it possible qualitative image of geometric shapes;
- gradual reduction of the cell with a solid reduces the number of elements of a cellular automaton, which speeds up process of calculating;
- allows to take into account the swelling process;
- makes it possible to calculate anybody undergoing deformation, as well as flexible body.

The developed algorithm is a fairly resource-intensive in terms of time, but the removal of cells from the solid in the course of dissolution allows to accelerate process of calculation. However, increasing the productivity of calculation is a priority. Therefore, the apparent prospect is the use of parallel computing by means of CUDA technology.

[968]

Data analysis and modelling of a Fluid Catalytic Cracking Unit (FCCU) for an implementation of Real Time Optimization

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The Fluid Catalytic Cracking Unit (FCCU) is considered as the heart of a modern refinery and corresponds to one of the first conversion process units. In the FCCU large hydrocarbon molecules are cracked into smaller hydrocarbon molecules, generating high value products such as diesel, gasoline and petrochemical useful olefins. Several studies have been made on the modeling, simulation, kinetics, multiplicity of steady states, chaotic behavior, on-line optimization and control of FCC units. However, there are still large areas to be examined due to the complexity and to the economic importance of this process.

The catalytic cracking kinetics involves a large number of reactions that generate a complex reaction network, based in the large number of different kind of molecules in the hydrocarbon feed, therefore several models of the cracking kinetics have been proposed. One of the most successful modeling approaches is the lumping scheme which relies in the characterization of the hydrocarbon mixture and generates groups according to a range of boiling point.

A dynamic simulation of a fluid catalytic cracking unit (FCCU) was developed using a phenomenological industrial validated model. The FCCU model considers riser, regenerator and stripper systems, in which the dynamic is controlled by the resident time in the regenerator and it considers a detailed description of the cracking kinetics that occurs in the riser unit. A set of perturbation was applied in the model for obtaining a large quantity of dynamic data that allows studying the system.

A parametric study of the input variables was developed for the FCCU in order to define the most important ones in the system performance, these variables were the input to design, train and test a Dynamic Neural Network (DNN). The DNN model is considered as the virtual FCCU. Gaussian error and gross error was then added to simulate real data plant. As the phenomenological model, DNN was implemented in Matlab taking advantage of the specific tool available for this kind of model.

The measurements in the real systems are often corrupted with random noise, gross error and systematic errors. These errors can arise because of faults and malfunction in instruments, problems in the process such measurement bias, signal conversion noise, etc. Therefore, data processing is an important step before doing an optimization process to make the data free of errors. In this work, data from virtual plant were employed for studying strategies for processing of online data, considering steady state identification (SSI), gross error detection (GED) and data reconciliation (DR) to eliminate measurement noise. For SSI, wavelets methods were the selected one, while for GED and DR a simultaneous strategy based on robust maximum likelihood estimator.

The advantage of using a virtual plant that represents adequately the dynamic behavior of a real plant is the capability of a more realistic interpretation of the plant performance because of perturbations and characteristics of data error are completely known. This allows us to study different scenarios, analyze how it works with different changes in the system and evaluate data analysis strategies. The developed virtual plant will be employed for studying Real Time Optimization (RTO) strategies.

[971]

A hybrid discrete/continuous dynamic model of trayed tower hydraulics

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According to Kister (1997), modeling and simulation are to be blamed for an alarmingly increasing number of tower malfunctionings due to primary design problems. He specifically mentions the lack of convenient hydraulic modeling as one of the sources. A general model was proposed some time ago by Gani et al (1986) but, although it has been cited many times, it does not seem to have been followed up. Oriented to the numerical solution, it neglects the influence of vapor dynamics. Wittgens and Skögestad (2000) have stressed the importance (and the lack) of realistic and accurate hydraulic models, focusing on the design of control systems. Nevertheless, they do not consider entrainment or weeping since is not so important for that application. Can et al. (2002) state that current models cannot reproduce failure situations, and therefore are not useful for safety analysis, but they do not accurately consider the hydraulic behavior. Staak et al. (2011) have repeated the same criticism, and have derived a complex model focused on the reproduction of pressure relief. However, they define stage liquid holdup as a whole, without considering separate tray and downcomer holdups (and the important phenomena that derive from them). More recently, Luyben (2012) has repeated the same claim, focusing on tower heat exchangers but without actually deriving any new model.

This paper presents a compact hybrid discrete/continuous dynamic model of trayed tower hydraulics that can reproduce situations out of the normal operation regime, in contrast to available commercial models. It may be used for process control or operability analysis as well as safety assessment and post-mortem studies, since the model considers a broad scope of operating conditions, including abnormal situations such as dry trays or reverse flow in downcomers. Using a hybrid continuous-discrete set of equations based on conventional correlations and general equations, each tray is divided into three independently-modeled compartments. This modular approach results in a highly flexible model that enables de simulation of multiple types of tower configurations. The model has been implemented in the Jacobian (RES Group, Inc.) simulation tool but can easily translated to popular platforms such as gPROMS or Aspen Custom Modeler. This hydraulic model is actually a subset of a more complete one where energy and material balances are incorporated under equilibrium or rated-based schemes.

Simulations have been done with single-pass sieve trays. They show qualitative correspondence with expected results, and have revealed unexpected phenomena. For example, the model predicts oscillations around the dump point for trays in the stripping section during startup, before the steady-state seal is achieved, resulting in unsteady transient responses of the clear liquid height in the trays. Complex behaviors can also be observed for the vapor streams that leave the trays, related to the achievement of the downcomer seals. As a result, an escalated pressure build-up is observed during the startup operation. Also, the model predicts that a higher vapor-load is required for the bottom tray to reach the dump point than for the rest of the trays.

[976]

Application of the Lagrangian CFD Approach to Modelling of Crystallization in Stirred Batch Reactors Using the Smoothed Particle Hydrodynamics Method

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Crystallization phenomena in stirred reactors are influenced by local hydrodynamic conditions and these must be taken into account for successful process scale-up and optimization. In this work, the available state of the art grid-based CFD methods and advantages and disadvantages of their application to mathematical modelling of batch crystallization processes were analyzed. The benefits of the Langrangian meshfree methods were discussed and the Smoothed Particle Hydrodynamics method proposed as an efficient method for a rapid prediction of the global mean flow in stirred reactors. Various aspects of the simulation results were assessed: quality of the fluid prediction, computational requirements, existence of numerical problems and availability of crystal size distribution. The developed Smoothed Particle Hydrodynamics CFD model was successfully coupled with discretised population balance equations to model a cooling batch crystallization process. It has been shown that 200 additional transport equations resulting from the discretisation of the population balance leads to only 50% decrease in computational performance while the same problem is still almost intractable from the computational point of view using the grid-based CFD methods.

[984]

Model reduction in visual modelling

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Whilst we have used it for year, we only recently presented and thereby introduced a graphical modelling method, which we call visual modelling [1]. We have used this method for years for the discussion of the structures of process models and computer implementations over a series of PhDs [2][3] resulted in a industrial implementation based on which a company was founded.

We use the method for time scale separation as reported in [4]. Here we want to extend the discussion to model reduction. We shall choose a couple of example to demonstrate the descriptive power of the graphical method: distributed systems to networks of lumped systems, and consequent simplification of the resulting networks based on order-of-magnitude assumptions. This approach can for example be used to derive the equation for a ideally-stirred tank reactor or its brother the plug-flow reactor, but also more complex systems of reducing networks of lumped systems to a simpler version in which we balance the time constants over the nework by simple arguments.

Our computer-aided modelling project has two main goals [5], namely to generate tools for the design of internally consistent models an to change the focus from writing equations to thinking and reflecting on the dynamics of the process to be modelled in the context of the utilisation of the resulting model.

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[986]

Automatic reconstruction and generation of structured hexahedral mesh for non-planar bifurcations in vascular network

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The accurate representation of arterial vascular structure is necessary to perform computational simulation and study of disease status like atherosclerosis. Current methods for automatic mesh generation face limitation when applied to the large vascular network. Although unstructured mesh are widely used for computational hemodynamic to represent the complex geometry of blood vessels; parametric meshes offer more accurate results with lower-density meshes and faster computation. Parametric volume discretization is of great importance for getting accurate solution for wall shear stress and fluid structure interaction.

Our aim is to present an automatic methodology for subject-specific reconstruction of a parametric mesh for planar and non-planar bifurcations. This method is suitable for computational fluid dynamics and fluid structure interaction investigation of large vascular network.

In this study, we generated a subject-specific fully automated vasculature model from medical images and applied parametric meshing for generating surface and volumetric meshes. Least square with Cubic Bezier approximation has been used to represent curvature of vessel morphology; G1 continuity is forced between adjacent Bezier curves. At the bifurcation, separation points have been automatically determined and surrounding Bezier curves are generated as such surface mesh orthogonality is guaranteed. Surface mesh points are longitudinally ordered in cross sectional groups. To make volume mesh, each cross section is subdivided into twenty parts to form a butterfly pattern by isoparametric transformation and interpolation. The computational meshes can be separated into vessel wall and lumen which vary in thickness and mesh resolution for arteries or veins. Finally, we also developed a robust meshing algorithm to automatically index both the surface and volume mesh. This methodology can also be extended to circular, elliptical and more complex tubular cross sectional shapes.

The application of our method to generate a parametric grid allows for better representation and a more computationally efficient patient-specific simulation of hemodynamics of the large vascular network in the entire brain.

[987]

Developing surrogate models via computer-based experiments

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In recent years, it is becoming a standard approach to conduct computer experiments to investigate the relation between a set of factors with responses of a process. Advances in mathematical modeling techniques, algorithms for solving mathematical equations and computation power all combined have made the study of complex phenomena with large number of inputs possible which could otherwise have been unattainable with physical experiments. Unlike physical experiment, which is characterized by random error, the response obtained from computer based experiment is deterministic. That is, multiple runs of the experiment at the same set of input variables yields an identical observation (Sacks et al., 1989). For this reason, statistical theories (i.e blocking, randomization and replication) that are developed for physical experiments to address random errors cannot be directly applied to analyze simulation data (Fang et al., 2006). The deterministic models describing the process are developed from first principles and are often complex which requires high computation power. One of the main goals in performing computer experiments is, therefore, to find an approximate (surrogate) model which is computationally cheap with sufficient accuracy. In multi-scale simulation of materials, surrogate models are used to bridge the gap between the fine and the coarse scales, i.e. the microstructure information contained at the atomic scale is mathematically connected with bulk physical properties. But building metamodels for such system is a challenging task due to the fact that there are different spatial and temporal scales. In this study, atomistic simulations on a system of polyurethane (PU) polymer are conducted. Our approach is to construct metamodels through fitting the data generated from complex deterministic simulations instead of following the classical stochastic approach of developing surrogate models valid for data with measurement errors. Different techniques of model fitting are implemented and their comparison of estimating the actual response is presented.

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[996]

Systematic development of kinetic models for systems described by linear reaction schemes

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Kinetic models of chemical reaction systems provide fundamental information for chemical process design and optimization. The traditional approach to develop these models is to postulate a reaction scheme (network of chemical reactions) based on observed species, their concentrations and eventually some theoretical or heuristic considerations on plausible reaction pathways. On top of this reaction scheme, kinetic laws for each reaction step are established, and regression of experimental data is used to determine the corresponding kinetic parameters. If reasonable statistical adjustment is achieved, the overall kinetic model, comprising the initially postulated reaction scheme and the kinetic parameters estimated, is accepted. If not, modifications are usually introduced, either in the kinetic models and/or in the reaction scheme used to describe the system. Due to the nonlinear nature of the regression problems considered, the required modifications are often not clear (or unique), and tend to be dependent on the expectations of the modeler relative to the behavior of system. Clearly, this is not a systematic procedure and, as such, it does not guarantee that the most plausible schemes are examined; this is especially true when the number of species and consequently the total number of possible reaction schemes to be considered is not very limited.

The identification of reaction schemes is a topic addressed in the literature under different contexts, namely synthesis of optimal reaction pathways from available raw materials, identification of metabolic networks and modeling of catalytic reaction mechanisms. Despite these contributions, a systematic and well-structured methodology to develop kinetic models is still missing, in particular one that fully incorporates experimental data when examining alternative reaction schemes.

This paper proposal is centered on the development of a systematic methodology for modelling linear reaction systems, including the identification of the structure of the overall reaction scheme, and the detailed kinetic modelling of each reaction step, where models of incremental complexity can be derived and evaluated, according to the interpretative needs of this task. The viable solution space is exhaustively explored, extracting the maximum information from the available experimental data. When needed, additional experiments for the discrimination of alternative models will also be identified and proposed. Compared with the traditional approach, we separate the task of elucidation of the reaction scheme that describes the system from the need of (a posteriori) determination of the kinetic laws, avoiding the use of nonlinear regression techniques during the initial phases of application and, consequently, of many of the numerical problems associated, significantly reducing the number of possibilities that need to be tested during the development of these models. For this purpose, a phased approach for generation of reaction schemes and plausibility tests relative to the available experimental data is proposed. This methodology provides a generic and well-structured approach for the development of kinetic models. We demonstrate its application to a number of case studies from the literature in the modeling of catalytic reaction systems.

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[1023]

Rigorous Modeling, Simulation and Optimization of a Dividing Wall Batch Reactive Distillation Column: a comparative

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Reactive Batch Distillation Columns (RBDC) have been studied as a promising technology due to its dual functionality: separation and reaction. Reactive Continuous Distillation, is characterized by high energy consumption. An innovative solution to overcome this problem is the use of dividing wall columns (DWC), which have found appeal in the chemical process industry as they can separate more components in a single distillation unit, thus achieving cost savings by requiring single columns instead of two, and by a decrease in operation costs using a single condenser and reboiler. Modeling, simulation, and optimization of batch distillation of processes require dynamic models. Several solution approaches have been proposed for the optimization of dynamic models described by a set of differential and algebraic equations (DAEs). One of them has been developed by Biegler et al[1], in which the dynamic optimal control problem is approximated by a finite dimensional nonlinear program (NLP) through the discretization of all variables using finite elements with orthogonal collocation. In contrast to this approach another solution method is the Control Vector Parameterization proposed by Vassiliadis et al.[2] which relies on the iterative solution of DAEs in the space of the control variables.

In this study we address the optimal design and operation of a dividing-wall batch distillation column with chemical reaction. The dynamic optimization problem is first converted into a nonlinear programming problem by using finite elements and collocation points implemented in GAMS (General Algebraic Modeling System, 24.2.2). The control vector parameterization technique is next solved by using gPROMS (general PROcess Modeling System, 2004) which makes use of an SQP method. We consider the esterification of ethanol and acetic acid to produce ethyl acetate (as the main product) and water. For a given product purity, this work investigates how parameters such as vapor load (V), reflux ratio (RR) and batch time (tB) should be selected to maximize a profit function (P) for the case of a batch distillation column that is divided by a wall in the internal plates. A comparison is presented with a simple batch reactive column to determine the potential benefit in the implementation of the dividing wall in the batch column. We also present a comparison of the computational experience with the two solution approaches, orthogonal collocation and control vector iteration.

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[1027]

Theoretical modeling of (non)reactive residue curve maps for TAME synthesis system using MATLAB – SIMULIS Thermodynamics communication facility

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The representation and graphical visualization of the chemical components in the composition space is a powerful tool for the analysis and interpretation of process systems behaviour. Reactive distillation is a relatively new technique combining reaction and separation by distillation. Numerous applications are reported in literature, giving details on process design. However, no commercial software is providing tools for representation of reactive residual curve maps. Reasonable explanation can be provided by complex reaction kinetics which is not easy to implement in software. In this study, liquid vapour equilibrium in (non)reactive systems is calculated to build (non) reactive residual curve maps, using SIMULIS® Thermodynamics (from ProSim, France) as database and server for with different thermodynamic models and MATLAB to solve the mathematical model aimed to build (non)reactive residual curve maps. The communication between those software applications is ensured by a MATLAB toolbox provided by ProSim. Graphical facilities of MATLAB allow to make suggestive representations. The work consists in setting up the methodology and the mathematical models for (non)reactive residue curve maps for non-reactive and kinetically controlled scenarios.

As illustration both non-reactive and reactive systems specific to synthesis of tert amyl methyl ether (TAME) are presented. TAME is obtained by heterogeneous catalysis from isoamylenes and methanol. As a consequence, it is possible to evaluate the feasibility of separation by distillation for these systems, because the analysis involve the evaluation of feasibility for both classical reaction-separation scheme and for reactive distillation based scheme. For this system, separation/reaction processes feasibility is assessed with infinite/infinite analysis, evaluating the influence of pressure and Damköhler number. Multiplicity regions are detected for higher Damköhler values by checking the influence of the distillate flow rate.

[1045]

Alternative prediction models for data scarce environment

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Prediction of future unwanted events in a process plant operation is useful in managing process risks. However, such models are difficult to develop due to unavailability of data on process failures. A common approach is to map a prior knowledge onto an assumed distribution function to determine the posterior. This is the basis of the Poisson-Gamma model that requires only a single data point to predict the future. Another alternative is to assume a model order and employs grey modeling strategy. Using this approach, four data points are required to fit the grey model parameters, and hence provide the needed prediction. This paper compares the two models on case studies involving a CSTR along with the Bayesian-Grey model, which is an extension of the Grey modeling strategy. Results obtained pointed to the superiority of the Baysian-Grey model over the other two approaches. Limitations and practical issues in implementing these models are also discussed to put data-scarce modeling in practical perspectives.

[1058]

Multi-objective Optimisation of Crude Distillation System Operations Based on Bootstrap Aggregated Neural Network Models

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The importance of distillation columns continues to increase both in the traditional petro-chemical industry and in the sustainable sector with renewable resources and energy. The key role they play in the chemical and petrochemical industriesand the quest to make them more energy efficient has made distillation process a high priority for all stake holders in the industries. For instance there areabout 40,000 distillation columns in the US alone. These consume about 40-60%of the total energy usage in the chemical and petrochemical industries and 6%of the total US energy. Also, major cost of operation second only to the costof crude in the refinery is energy and 35% of these is consumed in the crude distillation unit. Usually the order of economic importance in the control of distillation column is product quality, process throughput and utility reductions and often traded off between them has to be made. This paper presents a new methodology for optimising the efficiency of the crude distillation unit without trading off the product quality and process throughput. The method uses a neural network based strategy for the modelling and optimisation of distillation columns incorporating the second law of thermodynamics. Second law analysis indicates how well a system is performing compared to the optimum possible performance and hence gives a good indication of the actual energy use of a process. Real time optimisation of distillation columnsis made feasible by using neural network models which can be quickly developed from process operation data. The computation time in neural network model evaluation is very short making them ideal for real-time optimisation.Bootstrap aggregated neural networks are used in this study for enhanced model accuracy and also provide prediction confidence bounds indicating the reliability of the model. Aspen HYSYS was used for the simulation of the distillation systems. Neural network models for exergy efficiency and product quality are developed from simulated process operation data and are used to maximise exergy efficiency while satisfying product quality constraints. In addition to the operation objectives, the model prediction confidence bound is incorporated in multi-objective optimisation to improve the reliability of the model. The standard error of the network prediction indicates it's reliability.There is great potential for energy recoveryin the analysed processes. The recoverable energy is a sum of internal and external exergy losses. The economic analysis of the recoverable energy reveals the energy saving potential of the method. It is expected that the application of the methods will aid the design and operation of energy efficient crude distillation column.

[1075]

Simulation of a 3D bioprinted human vascular segment

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The ultimate goal of bioprinting is the production of living and functional tissue and organs for transplantation in a reasonable time scale. To achieve this goal, the best process would be organ printing. It has the potential to surpass the classic solid scaffold tissue engineering as we can see in the following advantages: Automated approach that offers pathway for mass production of tissue engineered products; it enables creation of tissue with a high level of cell density; can solve the problem of vascularization in thick tissue; organ printing can be done in situ.

Organ printing is a computer-aided 3D tissue engineering of living organs with layer-by-layer deposition of tissue spheroids compounded by pre-sorted cells and hydrogel with principles of self-assembly. This process can be divided in 3 technological steps: i) Development of design files for organs; ii) Actual printing; iii) Post processing or organ conditioning and accelerated tissue and organ maturation.

Post processing or organ conditioning, accelerated tissue and organ maturation. This phase consists on accelerating the maturation process by creating an environment propitious for the organ growth. This environment must offer perfusion of fluids including nutrients and oxygen and other controlled physical properties.

This abstract presents an initial study about the maturation phase. It was adopted a clinical image of computer tomography (CT) of a human heart. A branch of this heart was selected and handled. This image was converted into a 3D virtual mesh able to be used in the simulations. Two conditions were considered: a 3D branch formed by spheres analogously to the tissue spheroids representing a fresh organ bioprinted and the second one taking into account the surface of the branches representing a more maturated structured.

Some analysis were executed in order to verify the fusion process which means that the spheres suffered fusion and the distance between them decreased at long the time. Moreover, the fluid behaviour through the spheroids under these conditions and the stresses caused during the maturation phase were analysed.

[1110]

Modeling fixed-bed multicomponent adsorption as an step to achieve ultra-low sulfur diesel

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The elimination of nitrogen-heterocyclic compounds (NHC) in diesel may be considered as a strategic pretreatment to HDS to achieve ultra low sulfur diesel (ULSD). It is known that NHC in HDS processes compete favorably with sulfur-heterocyclic molecules (SHC) for sites in Co-Mo and Ni-Mo hydrotreater catalysts, at typical HDS operating conditions [1,2]. On the other hand, it has also been found that not only NHC adsorb favorably on various solids supports, but also SHC can selectively be adsorbed on the same type supports [3,4]. This leads naturally to attempt the selective adsorption of both NHC and SHC in diesel prior to HDS, aiming to achieve ULSD conditions. Moreover, the selective adsorption of both NHC and SHC can be performed at mild conditions in temperature and pressure, and with no use of H2. With the purpose of analyzing this possibility, and aiming to learn about the transient operation behavior of the fixed-bed adsorber, we have develop a detailed model that describes the continuous non-isothermal operation of the fixed-bed during the adsorption and regeneration stages of a pilot-scale unit (L=3 m; D=0.30 m) for the desulfurization and denitrification of a diesel (flow=0.36 m3/h) containing 500 ppm of a mixture of NHC and SHC species, at 333 K and 2.3 bar. In the transient model, intraparticle diffusion is assumed to be Fickean, and the mass and heat balances for the interparticle fluid are described by convective and dispersive terms, using a Darcy equation to properly account for the flow velocity in the bed. The adsorption and desorption are assumed to follow Langmuir kinetics under no-equilibrium conditions, using a wide range of kinetic parameter values to characterize the multicomponent mixture. The simulation considers a continuous three-stage adsorption-desorption operation where the corresponding intraparticle concentration profiles, at selected axial positions in the bed, and the profiles for the interparticle fluid in the bed are calculated. Model predictions compared the adsorbent performance when using particles of different dimensions. The model was solved by orthogonal collocation on finite elements for the interparticle fluid phase (up to 80 elements, using 4 interior points with elements of equal size), orthogonal collocation (one interior point) for the solid phase, the tri-diagonal matrix, and a fourth order Runge-Kutta. The code was parallelized reducing from 3 to 5 times the CPU performance.

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[1131]

Computational fluid dynamics study of circulating fluidized bed riser at two different scales

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A two-dimensional (2D) numerical simulation of gas-solids flow in a circulating fluidized bed riser was performed based on the two-fluid model (TFM). The effect of some essential parameters, namely, specularity coefficient (φ), and particle-particle restitution coefficient (ess), was examined for one set of operating condition. A range of specularity coefficients from 0.1 to 0.0001 were investigated. When specularity coefficient is set to values of 0.001 and above gives axial solid holdup profiles that reasonably agree with the experimental data. Moreover, the effect of the elasticity of particle collisions showed that the high particle-particle restitution coefficients gave good quantitative agreement. It was found that the specularity coefficient has substantial effect on bulk flow. Further extensive validations were carried out to investigate the model accuracy for a wider range of operating conditions. The model was capable of predicting the main features of the complex gas-solids flow for different operating conditions. However, the model showed some discrepancy in predicting the bottom dense regions operating at high solid circulation rate.

Maria-Ona Bertran, Thomas Bisgaard and Rebecca Frauzem (Eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. 31 May - 4 June 2015, Copenhagen, Denmark

[1144]

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

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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.

Track 2. Mathematical Programming (Optimization)

[67]

A framework for hybrid multi-parametric model-predictive control with application to intravenous anaesthesia

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In this paper we present a framework for the development of hybrid multi-parametric model predictive controllers applied to intravenous anaesthesia. A step-by-step procedure is described featuring a piece-wise model for anaesthesia describing the induction and maintenance phase, a recently developed multi-parametric mixed-integer quadratic programming solver and a novel hybrid control strategy tested for a set of 12 patients.

[101]

Dynamic Chance-Constrained Optimization under Uncertainty on Reduced Parameter Sets

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Uncertainty is a crucial topic for the decision making process in almost every scientific field. Therefore, the correct implementation into optimization problems is vital. Herein, the chanceconstrained optimization approach is applied and compared with a standard Monte Carlo optimization on a CSTR model. The two approaches are expanded by limiting the number of uncertain parameters in the system with according subset selection strategies from parameter estimation studies. The idea here is that a high number of uncertain parameters does not add to a better description of a system. The uncertainty can be represented by a subset of uncertain parameters, which suffice to describe the system behavior. In this contribution, it is shown that the results, both for the chance constrained and Monte Carlo optimization approaches, are improved regarding result stability and control action indication. Additionally, it is discussed how the chance-constrained approach yields even better results regarding the objective function of the optimization problem and it is shown that the solution time is drastically reduced.

[104]

Synthesis of inherently safer chemical processes with modular process simulators under the Generalized Disjunctive Programming framework

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It is well-known that chemical plants increasingly pose many hazards that can harm human health, the environment and property, due to many reasons like raised population density near industrial zones or complexity and use of extreme operation conditions. Hazard identification and analysis techniques have been developed to reduce the frequency and consequences of accidents. The most common method to mitigate risk and its consequences is by adding layers of protection with safety devices. Even though these protective measures have been successfully applied, they increase the complexity of the process and do not eliminate the hazards. Alternatively inherent safety principles of minimization, substitution, moderation and simplification aim to eliminate or significantly reduce hazards from a process, rather than managing them with engineering control systems and procedures. The opportunity to incorporate inherent safety features is highest at the early stages of process design, where the degree of freedom for modification is still high. Particularly, in the flowsheet design stage, all the interesting flowsheet alternatives can be combined into a superstructure, which later can be optimized. Handling discrete decisions leads to a Mixed-Integer Nonlinear Programming (MINLP) problem. To take advantage of modular process simulators even for the case of structural flowsheet optimization, Navarro-Amorós developed a methodology that integrates modular process simulators under the Generalized Disjunctive Programming (GDP) framework. The development of GDP in the process system engineering (PSE) community has led to customized algorithms that exploit this alternative modelling framework.

The goal is the integration of the safety assessment with a hybrid simulation-optimization tool that exploits the synergistic combination of commercial process simulators with GDP formulations and their corresponding logic-based solution algorithms. It is formulated as a multi-objective problem that seeks simultaneously to maximize the profit and minimize the inherent safety index. The inherent safety of each design alternative is measured by the Dow Fire and Explosion index, which has been previously suggested as an inherent safety index by Kletz and also used by other authors as a safety metric. We have developed a modelling system in Matlab that interacts with Aspen Hysys (through COM interface) and commercial optimization solvers (trough TOMLAB). The modelling framework proposed does not require to rewrite the problem as an MINLP, allowing direct application of solution methods for disjunctive problems. To this aim, we have used a homemade implementation of the logic based OA algorithm with the special feature that also allows the use of implicit models (i.e., those models inside process simulators). The capabilities of the proposed framework are illustrated with a case study for the synthesis of a plant for methanol production. The superstructure comprises several alternatives for streams, tasks and process conditions, where each option exhibits different performance in terms of profit and inherent safety. The solution to this multi-objective problem is given by a set of Pareto alternatives that capture the existing trade-off between economic and inherent safety objectives. The solution provides valuable insights into the design problem, and are intended to guide decision-makers towards the adoption of more inherently safer process alternatives.

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Optimal Design of Thermal Membrane Distillation Networks

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Thermal membrane distillation (TMD) is one of the novel separation methods used in the process industry. It involves simultaneous heat and mass transfer through a hydrophobic semi-permeable membrane with the use of thermal energy to bring the separation of a feed mixture in two streams (permeate and a brine streams). Thermal membrane distillation has been applied mainly for seawater desalination; however, TMD can be applied for fruit juice concentration, treating wastewater, drug concentration, water distillation and ultrapure water production. TMD offers several advantages over the existing separation technologies including high rejection of ions, macromolecules, colloids and cells, also TMD requires average operating conditions for its operation (i.e., relatively low pressure and low temperature) and therefore low energy requirements.

Traditionally, the studies about this technology have focused on the performance of individual modules as a function of the material and configuration of the membrane, leaving aside the design of TMD networks to satisfy physical and design constrains, and without considering mass and energy integration. The objective of this paper is to develop a systematic approach to synthesize optimal TMD networks. Therefore, a structural representation is developed to embed potential configurations of interest, which can be a series arrangement, parallel arrangement, or a combination of both (for example the Christmas tree arrangement). The building blocks of this representation include TMD modules, pumps, heaters, and condensers. A rigorous mathematical formulation is developed as a mixed-integer nonlinear programming model to transform the design problem in an optimization formulation that seeks to minimize the cost of the system. The objective function takes into account the capital and operating costs for the TMD network. The proposed optimization model was applied to two case studies for seawater desalination and syrup dextrose concentration, where the optimal network structures as well as the operating conditions were determined. The results obtained show that the proposed model yields better results than other configurations, and that these results can satisfy feasibility and design constraints. Also, the results showed economic benefits associated to the sales of fresh water and energy savings.

[127]

Multi-cut multi-column cross decomposition for stochastic mixed-integer linear programming

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Two-stage stochastic mixed-integer linear programming (MILP) problems can arise naturally from a variety of process design and operational problems. These problems, though usually large-scale MILPs, are well structured, and they can be solved efficiently by Benders decomposition (BD), or sometimes Dantzig-Wolfe decomposition (DWD) and Lagrangian decomposition (LD) as well. In addition, Van Roy showed that a cross decomposition method that combines BD and LD could be more efficient than BD[1].

Recently, the authors have developed a new cross decomposition method that combines BD and DWD for solving stochastic MILPs, and it has been shown that this cross decomposition method is faster than BD for a supply chain network design problem [2]. In this paper, a variant of this new cross decomposition method is developed, which generates multiple cuts or columns in one Benders or Dantzig-Wolf iteration. Just like that a multi-cut BD converges faster than a classical BD [3], the multi-cut multi-column cross decomposition method can converge faster than the plain cross decomposition method. It will be proved that the method still guarantees finite termination with an optimal solution, when the multi-cut multi-column strategy is adopted.

The case study of a bioenergy and bioproduct supply chain optimization problem shows that, while the plain cross decomposition is about 50% faster than Benders decomposition, the use of multi-cut multi-column strategy can further improve the computational efficiency by up to an order of magnitude.

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[143]

Efficient ant colony optimization (EACO) for solvent selection using computer aided molecular design

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Efficient ant colony optimization (EACO) is a new metaheuristic optimization algorithm for tackling linear, nonlinear and mixed integer nonlinear (MINLP) programming problems. In this work, a solvent selection optimization problem modeled based on a novel computer-aided molecular design (CAMD) methodology is optimized using an EACO algorithm. The molecular design problem is formulated as an MINLP model where a solvent solute distribution coefficient is maximized subject to structural feasibility, property and process constraints. The capability of the proposed methodology is illustrated through a case study of an extraction of acetic acid from waste process stream by liquid-liquid extraction. Environmentally benign new solvents with better targeted properties are proposed.

[192]

An approach to optimize multi-enterprise biofuel supply chains including Nash equilibrium models

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In recent years the energy production from biomass has become increasingly important, both for security reasons (particularly, the exhaustion of oil reserves) and environmental concerns related to climate change. Biofuels have risen quite a lot of interest in the transport sector as alternative substitutes to fossil fuels. In particular, corn-based bioethanol has been dominating the market [1]. However, there has been a general lack of focus on the multi-enterprise biofuel supply chain optimisation which constitutes a complex problem of decision making connected to the operational management of the supply chain when it is required to simultaneously optimise operational decisions as well as profit allocation mechanisms in supply chain optimisation, namely material transfer prices and revenue share policies among the supply chain stakeholders [2-3]. Furthermore, the economics of bioethanol from first generation technology strongly depends on the feed stocks supply costs [4-5]. Therefore, it is crucial to introduce proper market mechanisms to satisfy the interests of different parties to address possible business partnership scenarios among feedstock suppliers and biofuel producers, which the price transfer policy is an intuitive and efficient method to create a fair, optimised profit distribution in the biofuel supply chain using the Game Theory as powerful tool in the decision making under such conditions.

This work aims at incorporating a game-theoretical Nash-type model approach within a Mixed Integer Linear Programming (MILP) framework in order to optimise a fair profit distribution between members of multi-enterprise supply chains. Under this scheme, the system behaviour is tested in a case study representing the dynamic evolution of a bioethanol supply chain under increasing biofuel demand [6]. Model decision variables include the biomass production for each site and its supply strategy, the location and capacity of each biorefinery in the network comprising the transport logistic of the product. As a key factor corn price dynamics is introduced in this approach which is also the major variable in this optimisation problem in order to maximise the financial performance of the actors involved over a time horizon. The proposed method is illustrated by a case study on a corn-based biorefinery supply chain network design in Northern Italy.

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Price based coordination for shared resource allocation in an integrated petrochemical site

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This paper presents a price based coordination algorithm for large-scale dynamic interconnected systems consisting of dynamic subsystems that are coupled by various shared resource constraints. This structure of interconnected systems is typical for large chemical plants.

In the petrochemical industry, a hierarchical automation structure has been implemented in many plants, ranging from the basic automation over the regulatory control layer (often MPC controllers) to real-time optimization and plant-wide production planning. While a full integrated optimization of the set-points of a large complex may be feasible in principle, the size of the problem, the vulnerability to missing data and above all the management structures of the plants often favour a distributed solution where local optimizers (or managers) are responsible for the operation of individual units and the global coordination has to be achieved by suitable mechanisms. E.g., different units may be operated by different business units of a company or even by different companies in a chemical park who do not want to make all details of their operation and of the cost and profits transparent.

A characteristic feature of processing plant complexes is that the units are coupled by networks of utilities, e.g. steam, cooling water or hydrogen. In these complex networks, the units can act as consumers and producers of resources. The utilization of these shared resources has to be coordinated between the distributed structures in order to fulfill the global demand-supply constraints for each network. The hold-ups of the networks often are quite small compared to the production/consumption rates, so the networks provide only limited buffers. The optimization problem is defined as a reference tracking problem with an additional constraint that the total amount of supplied and consumed shared resources must be zero.

For the computation of the optimal solution for a complex network of interconnected units, we propose a hierarchical coordination algorithm based on a subgradient method that can be implemented in a distributed fashion, is simple to implement and has convergence and performance guarantees. One possible way to implement the optimal solution for the overall system without detailed knowledge of the models and of the cost structure of the subsystems is by the implementation of a price based coordination algorithm. While this method has been extensively investigated for static subsystems and for scheduling problems (with mixed success), price based coordination of continuous coupled dynamic subsystems has hardly been addressed. This paper presents an implementation of a price coordination scheme for continuous dynamic subsystems of a large complex that are coupled by constraints on the connecting networks. The algorithm adjusts the price trajectories for the predicted demand and supply patterns using model-based predictions for a defined horizon. Similar to MPC schemes, in every time-step only one element of the price vector is implemented. Then, in order to take disturbances into account, the price trajectories are calculated again in the next step resulting in a receding horizon scheme. The predicted prices and the predicted demand and supply patterns of the shared resources are used for the initialization in the following sampling time.

The proposed approach is applied to a large-scale plant model with six units and three coupling networks provided by INEOS in Köln.

[240]

Optimisation of process parameters with simultaneous consideration of energy efficiency measures

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Energy efficiency is a mayor global concern of latest research as well as industrial application. Limited fossil fuels lead to constantly rising energy costs. Tightening environmental regulations necessitate the reduction of CO2-emissions and waste water generation. All these issues underline the importance of the efficient use of energy and resources likewise. In this context process integration and optimisation are powerful approaches that allow process industries to increase their effectivity and profitability.

In order to advance the state-of-the-art technology and accelerate a move to low carbon manufacturing industries several research projects were funded by the European Commission via the seventh framework programme. One of those projects, namely EFENIS, aims for a fundamentally improved process integration by applying novel methods of total site targeting, heat recovery, intensified heat transfer, CO2 and waste water management. The EFENIS project is composed of 17 partners including 10 academic institutions and 7 industrial companies.

Within EFENIS an efficient and sustainable workflow for assuring a long term validity of total site analysis results will be developed and implemented into a decision supporting software tool. This Energy Integration Manager has to be based on sophisticated interfaces between state-of-the-art process simulation, process optimisation and data management. The operability of this software tool will be tested with datasets and process models of actual operating industrial plants. Close cooperation with industrial partners within the EFENIS consortium will ensure the capability of the decision support tool to handle the complexity of real life total site integration projects.

Utilizing the above mentioned software solutions for process simulation enable the parallelisation of process integration and process optimisation as a simultaneous design step. This concept is in contrast to the traditional workflow of sequentially doing the heat integration after finishing the process design. In terms of heat integration, the design of a comprehensive heat exchanger network will be the focus. In terms of process optimisation, the optimal parameterisation of relevant process variables is the core objective.

In the presentation a concept of a genetic algorithm for process parameter optimisation using a multi-criteria solution approach is shown. The impact of process parameters on heat integration measures will be presented via suitable pareto illustration. As a case study a process for the synthesis of dimethyl ether from methanol is used.

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[246]

Comparison of two different implementations of optimizing control for a continuous polymerization process in a tubular reactor with side injections

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From a process engineering point of view, the goal of the control system is to derive the process to an operating point which yields the maximum economic profit. Optimizing control has shown its capabilities for this purpose. This scheme takes an economic measure of the process as the cost function while the purities of the final products are considered as constraints. This formulation, however, leads generally to non-quadratic optimization with many decision variables subject to the dynamic model of the process and is computationally demanding. Limited computation power and lack of efficient optimization algorithms have pushed most of the previous works in this field to the lumped-parameter systems. Hence efficient implementations of the optimizing control have to be investigated to apply it to the distributed systems. In this contribution we study the potential of optimizing control for a continuous polymerization process in a tubular reactor with multiple side-injections of monomer. Five manipulated variables, namely four side injections of the monomer along the reactor and a uniform jacket temperature, are available. The molecular weight of the produced polymer and its residual monomer are measured at the reactor outlet. The configuration of this reactor which imposes large time delays between the inputs and the measurements at the reactor outlet and the lack of intermediate measurements, as well as the complex polymerization reaction with sharply changing system states, makes the implementation of the optimal control for this process challenging. In order to transfer the rigorous pde model of the process to an ode system without the need of fine discretization grid, we have used the weighted essentially non-oscillatory scheme (WENO) to discretize its spatial domain. Using this scheme, the ode system of the process has a dimension of 1600 which is 25 times smaller than the one that would be produced using the finite differences to discretize the spatial domain for the same simulation accuracy. The controller maximizes the product throughput subject to the product constraints. We first formulate the optimal control problem using a control vector parameterization scheme which has the advantage that the obtained optimization problem has only a few decision variables and is favorable for the numeric optimizer. On the other hand, a numeric integrator must simulate the process model to compute the optimization constraints (product constraints) which makes the computation of the sensitivities of constraints difficult and slow. As the second approach, we formulate the optimal control problem as an NLP problem using a full-discretization scheme and the orthogonal collocation on finite elements. This formulation does not include explicit numeric integration and the sensitivities of the product constraints are provided analytically. However, a large NLP problem, for our case including more than 52,000 variables, results. We have formulated the NLP problem with different number of collocation points and finite elements and investigated their effect in the performance of the controller. Two implementations are compared in terms of the objective values and computation times for different formulation of the cost function and the constraints (hard or soft) and different control horizons.

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Optimization of split fractions and cleaning schedule management in heat exchanger networks

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Fouling is a non-negligible problem to heat exchange operation, because it will cause sustained reduction to the overall heat transfer coefficient due to the growth of deposit over heat transfer surface of heat exchange equipments. Implementing regular (routine) cleaning is a recommendable means to remove fouling. As heat load distribution of parallel branches is related to split fractions, this paper presents an approach to arrange the cleaning schedule with having split fractions optimized concurrently. To avoid the numerous integer decision variables produced in time discretization method, the maximum allowable fouling resistance of a heat exchanger is taken as the optimization variable in this study. Then the proposed method is formulated into a Mixed Integer Nonlinear Programming (MINLP) model, to aim for the minimum operating cost of an existing HEN. At last of the study, an example from literature is studied, and the effectiveness of the method has been demonstrated by the proper results.

[336]

A cost targeting method for estimating investment on heat exchanger networks for collection of industrial excess heat

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Large amount of heat at medium and low temperatures is often dispersed from industrial plants to the environment by means of water or air cooling. This heat can be recovered for different purposes such as for reducing on-site fuel demand by heat exchange with cold process streams, for exporting heat to nearby urban areas by district heating networks, or for producing electricity by means of organic Rankine cycles. A practical way to avoid extensive process retrofit and to avoid potential hazard of process leaks is to use heat collection systems based on water or oil loops. Cold water or oil is used to cool process streams thus collecting heat at one side of the loop. At the other side, the hot medium can be used to provide heat e.g. to cold process streams, to a district heating network, or to a centralized power plant. At the Heat and Power Technology division at Chalmers, feasibility studies have been recently conducted on heat recovery and excess heat export from a petrochemical cluster located in the Swedish West Coast. An interesting point of investigation is to establish the amount of heat to recover in order to maximize profitability of the new installation. Equal amounts of heat can be recovered from different set of process streams and their arrangements. In addition, different temperature levels of the heat collection system allow more or less heat to be recovered. Following the objective of progressively automatizing our calculations, in this work we tackle the first of the two problems that is finding the optimal combination of process excess heat sources for a different amounts of excess heat recovery. For this purpose a genetic algorithm based optimization tool is used. Different candidate arrays of hot process thermal streams are generated and the corresponding investment cost is estimated through a Pinch Analysis based procedure. For a given stream set, the cooling profile (temperature-heat load) is built by aggregating the stream heat contributions at different temperature levels. The investment on heat exchangers is estimated considering vertical heat transfer between hot process streams and the heat collection medium in counter-current arrangement considering an opportune value of the minimum temperature difference. The genetic algorithm based optimization progressively evolves the population of candidate stream arrays and eventually sort out a Pareto curve showing the dominant front of combinations of process excess heat sources that should be chosen to minimize the investment in a wide range of excess heat recovery. The analysis is conducted for four plants belonging to the petrochemical cluster used here as study case. The results are finally compared with results from previous investigations in which the process excess heat sources were chosen based on their incremental contribution to the heat recovery target. This allows us to derive some engineering principles that can possibly facilitate future investigations.

[364]

Solution of two-stage stochastic scheduling problems by stage decomposition and ordinal optimization

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Chemical batch scheduling problems in the literature in most cases are solved for nominal problems where the equipment, recipes and production orders are given and fixed. In reality, however, scheduling has to be done under significant uncertainty about yields, availability of equipment and personnel, and especially varying demands, rush orders, cancellations etc. Scheduling problems can be modeled by two-stage stochastic mixed-integer linear programs, where the uncertainty is modeled by a discrete set of scenarios and the option of recourse decisions that react to the actual evolution is represented. If several uncertainties are included, the number of scenarios grows rapidly. With an increasing number of scenarios the resulting MILP problems become computationally very hard to solve in a monolithic fashion, making it impossible to apply this approach to realistic problem sizes. Decomposition techniques and/or (semi)heuristic approaches can then be used to find good solutions in reasonable computation times.

In a previous approach stage decomposition was successfully applied to solve two-stage stochastic scheduling problems, where the first stage problem is solved by an evolutionary algorithm, while the second stage subproblems are solved exactly by a solver for mixed-integer linear programs. Later this idea was improved in by the use of systematic initialization techniques. This implies that for each tested solution for the first-stage variables, all scenario subproblems are solved to optimality, so the computation time increases at least proportional to a multiple of the number of scenarios.

In this contribution, a new idea for solving large-scale two-stage mixed-integer stochastic programming problems that arise from chemical batch scheduling under uncertainty is introduced based on stage decomposition and the principles of Ordinal Optimization (OO): 'Order is easier than Value' and 'Nothing but the best is very costly'. According to OO it is easier to create a ranking of multiple solutions than evaluating their exact values. Hence a heuristic evaluation might be used to find a correct ranking of solutions (with a small error). Applying this idea to two-stage stochastic programming solved by stage decomposition, we replace the time consuming calculation of exact solutions for all scenario-related subproblems, which were used before to rank different first-stage solutions, by a non-exact evaluation, allowing us to find good solutions for very large problems with a large amount of scenarios in relatively short computation times.

We evaluate our approach by a case study of a chemical batch plant for the production of expandable polystyrene. Different evaluation methods for the ranking of the solutions are compared to the true ranking provided by an exact evaluation of the second stage problems to validate the assumption that a heuristic evaluation can be used to gain a correct ranking with only a small error. Afterwards the algorithm is tested experimentally and compared to standard methods.

[388]

Ellipsoidal Arithmetic for Multivariate Systems

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The ability to compute tight enclosures of the image set of nonlinear functions is pivotal to many methods in such areas as global and robust optimisation, reachability analysis and uncertainty analysis. For real-valued, factorable functions, interval arithmetic [1] provides a natural way of computing such enclosures, since the image set of any continuous function is itself an interval. In practice, an interval enclosure can be obtained by traversing a directed acyclic graph (DAG) [2] of the function in order to bound its atom (unary or binary) operations recursively and as tightly as possible. Although simple, this approach suffers two main limitations, namely the dependency problem and the wrapping effect. The former happens when multiple occurrences of the same variable, e.g. in a complicated function expression, are treated as if they were independent from each other. The latter is due to the fact that the image of an interval vector under a vector-valued function, even a linear function, is generally not an interval vector itself, thus leading to overestimation in enclosing that image set with an interval vector.

The main focus of this paper is on constructing ellipsoidal enclosures of the image set of factorable functions. Here, the host set is assumed to be contained within an ellipsoid and the problem consists of computing another ellipsoid that encloses the image set of a nonlinear factorable functions f: IRn -> IRm. Analogous to interval analysis, our approach involves traversing the function's DAG. The propagation of the ellipsoid proceeds by adding an extra dimension (lifting) for every atom operation in the DAG. For efficiency, the (symmetric) shape matrices of the lifted ellipsoid is stored in sparse format and every atom operation corresponds to a sparse update of the shape matrix – We make our implementation freely available as part of the software package MC++ (https://projects.coin-or.org/MCpp). In essence, the proposed approach is similar to the construction of polyhedral relaxations using a decomposition-linearization approach [3,4], with the added benefit of a well-developed ellipsoidal calculus [5]. Keeping a trace of previous operations in the shape matrix helps capture possible dependencies in the function. Also, the fact that ellipsoids are invariant under affine transformation contributes to mitigating the wrapping effect compared to interval arithmetic. We present theoretical and numerical results regarding the quadratic Hausdorff convergence of the ellipsoidal enclosures and present applications in the field of chemical process control.

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Reduced model trust region methods for embedding complex simulations in optimization problems

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In recent decades, significant advances have been made in the area of gradient-based nonlinear optimization. However, for a practitioner, fully open, differentiable models required for these algorithms may not be available for all parts of a system. For example, it may be desirable to model a unit operation with a computational fluid dynamics simulation (CFD), but this is computationally expensive and derivative information may be unavailable. A common approach to include complex models in optimization problems is to construct reduced models (RMs, also known as surrogate or meta-models) that approximate the behavior of the simulation with a simple algebraic form. Because the RM easily provides derivative information, the RM may be substituted into the original problem for use with modern gradient-based solvers.

In this work we use trust region concepts from nonlinear programming to systematically construct a series of local RMs to solve overall problem. If these reduced models are constructed in order to satisfy the "fully linear property" described by Conn, Scheinberg, and Vicente, convergence can be guaranteed under mild assumptions. Popular sample-based reduced model techniques such as polynomial regression and Kriging interpolation are suitable choices for reduced models.

Two methods are presented for handling constraints. First, a penalty function method is presented that essentially recasts the problem as an unconstrained derivative free optimization problem. Secondly, a filter-based method is developed based on the ideas of the trust region filter algorithm of Fletcher et al.Penalty functions use a combined metric of objective function decrease and feasibility, whereas a filter borrows concepts from multi-objective optimization to handle these concepts separately. In doing so, the filter is better able to exploit the structure of the full system.

The performances of the trust region RM-based optimization methods are tested on two flowsheet optimization examples: the Williams-Otto process and the ammonia synthesis process. In each of these processes, the reactor is considered as a complex system and will be represented with a RM during optimization. The results indicate that the filter method is able to reduce the number of function calls to the complex model by nearly an order of magnitude while still obtaining the correct solution. This is largely attributed to the filter method's superior capability to handle equality constraints.

Although the theory only requires any RM satisfying the fully linear property, the type of RM and methodology used to construct it can have a strong effect on practical performance. We discuss the advantages and disadvantages of three RM construction schemes. The best performing RM is a linear fit, which also includes the well-known finite difference gradient estimate, among her possibilities. This generalizes the concept of using good derivative estimates whenever available.

[436]

Energy Supply Chain modeling for the optimisation of a large scale energy planning problem

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The energy planning problem has taken very emerging importance during the last years mainly due to the pressing issues that need to be taken into account such as economic, environmental and social considerations, while at the same time the technology supports many more options and alternative solutions in the design of the energy supply chain.

Following that, energy and fuel Supply Chains (SCs) seem to be re-examined and reconsidered under more integrated approaches having their origin in the production management, i.e. energy SC management, proving their technical and economic viability. In this context, the present work is a continuation of our integrated research in energy supply chains and attempts to apply the methodological framework that has been developed in a wider geographical area.

More specifically, the present work applies an RTN based novel representation of the Energy Supply Chain, along with the mathematical programming optimization model in order to analyse and model the country's energy planning problem with special considerations to the fuel mix and the contribution of various energy sources in a global scale.

Independently of the results obtained, the present work's added value is mainly focused in the development of the model and the analysis of various energy planning scenario and intends to be a very valuable tool for the decision makers in the design of the energy supply chain taking into account on a rational basis all the parameters that govern the solution of such a complex and critical problem.

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Optimization of LNG supply chains

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The continuously rising energy consumption in the world and the increased focus on environmental aspects of energy consumption are causing a demand for a cleaner fuel to replace existing, polluting, fuels such as fuel oil and coal. Natural gas has propitious environmental properties and large remaining reserves which makes it to a suitable fuel candidate for meeting the demands required of a fuel in the future.

Natural gas is traditionally transported from gas fields to consumer sites with pipelines, but the total cost of pipeline transportation is economically unfeasible for long distances. Thus, many areas with intensive energy consumption are left without natural gas due to their geographical location. The best way to introduce natural gas to new, scattered, areas is by transporting it as liquefied natural gas (LNG). LNG is produced by cooling natural gas to below -162 °C. In its liquefied state, natural gas can be shipped from a large import terminal to consumers through a network of smaller satellite terminals with a combination of sea- and land-based transports.

Building a small-scale LNG supply chain network is expensive and capital intensive and the choice of efficient satellite terminal locations is an arduous task. This paper presents a mathematical model to aid decision making in the LNG supply chain design, with the focus on satellite terminal placement and inter-terminal transportation. The model, which considers distribution of LNG to consumers from multiple supply terminals through multiple satellite terminals by a heterogeneous fleet of ships, utilizes mixed integer linear programming for finding a supply chain structure that minimizes costs associated with fuel procurement. As LNG is at cryogenic temperature, special aspects in the transportation and handling must be considered. The performance of the model is illustrated by case studies, where optimal supply chains of LNG distribution for different kinds of geographical regions and different demand structures are designed. By sensitivity analysis the effect of different central parameters on the optimal solution is investigated.

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Metaheuristic Techniques for the Optimal Design of NGL Pipelining

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The rising price of fuels and the associated increasing costs of transportation boost research in the exploration of strategies that aim at exploiting and transporting dormant energy sources. Cost-effective solutions are required to cope with volatile economies. In this work a preliminary design of an optimization model is presented. The approach consists in finding the most convenient piping layout to transport NGL (Natural-Gas Liquids) through a country subjected to an unstable economy. NGL revenues and cost factors –such as construction, operation and power expenses– are discounted by using the Net Present Value technique. This method ensures an accurate comparison among different pipeline networks. Namely, diverse payback flows and operative costs are carefully contrasted along time. The effect of macroeconomic volatility on long-term investment decisions is considered by applying to the discount rate an econometric technique known as Generalized Autoregressive Conditional Heteroskedasticity in Media (GARCH-M).

The model also serves to find the most suitable location of the concentrating nodes, i.e. the sites where NGL should be temporarily stored on its way to the processing plants. The problem is solved by means of specially developed metaheuristic algorithms. Metaheuristic techniques founded on trajectories, such as Simulated Annealing, are compared with population-based methods, like Genetic Algorithms.

The most promising design approaches are assessed. Their performance and robustness are tested through various metrics, such as the amount of required fitness-function evaluations, and the computing times until convergence. The evaluation of the solution quality is carried out from both computational and engineering viewpoints. The analysis is applied to the design of a real-world pipeline network. NGL coming from gas fields located in Santa Cruz province (Argentina) are sent to the processing plants, which are potentially placed at either Río Gallegos or Puerto Santa Cruz. Thanks to the resulting model, an adequate pipeline network layout can be achieved.

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Deterministic Global Dynamic Optimisation using Interval Analysis

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Dynamic optimisation problems arise in many applications in chemical engineering, e.g., the determination of optimal operating profiles, the formulation of process control strategies, the parameter estimation for model development, etc. There is an interest in obtaining the global optima, i.e., the absolutely best solution, for these problems since it often offers substantial improvement compared to locally optimal solutions. Furthermore, in safety critical applications it is important to ensure that the behaviour of the process is within (possibly prescribed) safe limits.

Currently, the main bottleneck in the deterministic solution of global dynamic optimisation problems is the computation of tight bounds on the solutions of the ordinary differential equations (ODE) related to the system. Moreover the exact solutions of the problem are required to be contained in the computed bounds at all times. Also for the dynamic global optimisation problem it is necessary for these bounds to be obtained for sufficiently large time horizons, and for interval parameters and initial conditions to be as wide as possible.

Several are the methods which have been proposed for the solution of global dynamic optimisation problems. Most of these methods rely on sequential approaches in which an ODE solver and a spatial branch and bound framework are used. However, none of these approaches takes into account uncertainty in the system parameters and cannot provide guaranteed safe bounds. In this work, the global dynamic optimisation problem is addressed using a sequential approach. The dynamic set of constraints (ODEs) is solved using an interval Taylor series method with interval contractors and a spatial branch and bound framework is used as the optimisation routine. The key contribution of this work is the introduction of uncertainty in the system parameters as interval values and therefore the determination of upper and lower bounds on the optimal trajectory. The approach presented here is illustrated with a case study of a chemical reactor.

[484]

Simultaneous analysis and design applied to optimal control problems on nonlinear dynamic systems

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A Modelica-based package has previously been reported on which allows unit-operation based simulation of chemical engineering systems. Models built using this system can be flattened into a single system of differential-algebraic equations (DAEs). This allows automatic techniques to be used to solve the system using collocation methods. Recent advances in optimisation solvers allows these equality constraints to be applied while solving an additional optimisation problem. We show how a chemical system can be modelled in the environment, how an optimal control problem can be formulated using this system model and how the optimal control problem can be solved using a single solver invocation. The benefits of the system are that the Modelica environment allows intuitive modelling, that the tools employed provide a mostly automated workflow and that the solution of the optimal control problem is faster using the simultaneous approach than using older techniques involving solving the DAE many times while the optimisation proceeds.

We also show an extension to the system which allows for spatial derivatives to be included in the formulation. By meshing simultaneously in both the time and space dimensions, the mesh can be refined in a way that reduces the total number of equations used without giving up any accuracy.

[489]

Separation process optimization under uncertainty by chance constraint programming with recourse

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Uncertainties in process variables are unavoidable when considering the design and optimization of separation processes. There are two main sources of uncertainty: 1) uncertain internal process parameters such as the feed rate, operating temperature and pressure, etc; 2) uncertain external process parameters such as the product demands (which may change), raw material and product price fluctuations, and uncertainties in the supply of utilities. Conventional deterministic methods normally lead to conservative designs. To obtain solutions with greater potential a methodology for optimization of separation systems under uncertainty should be developed.

2-stage stochastic programming with recourse (SPR) and chance constrained programming (CCP) are important approaches for optimization under uncertainty. SPR is relatively strict and reliable, while CPP is fairly simple and direct but involves some risks.

A new methodology for chance constrained programming with recourse is proposed in this paper. Uncertain variables are classified and treated using CCP and SPR respectively based on their characteristics. The effect of some uncertain parameters are expressed as penalty terms and added to the optimization objective, while other uncertain parameters are treated using CCP which allows decisions to be made which violate constraints according to certain probabilities based on the levels of confidence.

Solving models in this way, the chance constraints are transformed into equivalent deterministic constraints in the multivariate integration and penalty terms in the objective are discretized using a revised Monte Carlo method. The modified Benders decomposition algorithm used with SQP is an effective strategy which is used here to obtain an optimal result.

A case study investigating the optimization of a 1-hexene separation process is used to illustrate the methodology.

[492]

Optimal design of a Reverse-Forward osmosis hybrid system for the shale gas wastewater treatment

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The shale gas revolution with a production in the US of 8.6 trillion cubic feet in 2013, and above all, a estimation of 7800 trillion cubic feet of technically recoverable shale gas worldwide, has a crucial repercussion in Process Systems Engineering (PSE) community. Natural gas is the cleanest fossil fuel, and can serve as a bridge in the transition to a clean-energy future, especially for moving away from coal-powered energy production. Nevertheless, shale gas extraction is not free of problems. Indeed, hydraulic fracturing demands large amounts of water, on average 19000-23000 m3 of water per well. Consequently, high volumes of wastewater from shale gas well pads are generated.

The water that returns to the surface from a shale gas well is classified into 2 types, flowback and produced (or formation) water. The flowback water refers to the outbound water flow during the first weeks, which is characterized by high volumetric flowrate and relatively low total dissolved solids (TDS) concentration. The water that returns to the surface after the initial weeks is called produced water, which has high salinity and low flow rate. Constituents of concern in flowback and produced water include total dissolved solids (TDS), total suspended solids (TSS), organics, hardness, metals, biological load, and naturally occurring radioactive material (NORM). These contaminants can be removed by a combination of mechanical, chemical and thermal technologies.

Among the category of desalination technologies, reverse osmosis (RO) is often considered as a solution for reducing TDS concentration in flowback water. However, RO is an energy-intensive process because of the high pressure required. In the last few years, Forward Osmosis (FO) has emerged as an alternative membrane technology for water purification and desalination. FO is a natural osmosis-driven process involving a semipermeable membrane and a draw solution. A step forward in membrane systems consists of coupling FO with RO to generate a synergistic multi-barrier hybrid system for water treatment. Indeed, the combination of both technologies have been already included in the superstructure for the optimal design of a seawater desalination plant.

In this work, we integrate FO in the whole set of available water treatment technologies of a shale gas facility. By two sets of mixers and splitters, the superstructure proposed comprises all possible connections among the RO and FO units, flowback water mixer and rejected water collector that account for the alternatives of interest. We handle the optimization problem under the Generalized Disjunctive Programming (GDP) framework. We formulate the synthesis of a shale gas wastewater treatment plant as a multi-objective problem that seeks simultaneously to minimize the specific total cost ($/m3 of flowback water treated) and the specific freshwater consumption (m3 freshwater consumed/m3 of flowback water treated).The capabilities of the FO/RO Hybrid treatment system are illustrated with a case study for a shale gas wellpad with a flowback water ranged between 200 and 3000 m3/day. The solution (i.e., a set of Pareto points) captures the trade-off between the cost and water consumption indicators and shows how different topologies of the wastewater network arisen for each Pareto alternative. The solution also highlights the suitability of FO/RO hybrid system for decreasing the freshwater consumption and simultaneously offers a solution to the treatment of the formation water.

[495]

Optimal operating policies for synthesizing tailor made gradient copolymers

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The discovery of the controlled polymerization of styrene in the presence of 2,2,6,6-tetramethyl-1-piperidynyl-N-oxy (TEMPO) ushered the research of the promising controlled radical syntheses. Since then, TEMPO has been extensively studied and applied thanks to its low cost, commercial availability and lack of environmental issues. Even though operating temperature needs to be relatively high (> 100ºC) and the achieved control over molecular structure is not as precise as with other controlled polymerization techniques, the advantages of TEMPO mediated polymerization still make it an appealing method to obtain high value materials in an simple, economic and environmentally friendly way. Furthermore, the produced polymers lack the potential to develop foul smells or change color.

In many applications, gradient copolymers could represent a cheaper alternative than their block counterparts due to the relative simplicity of the synthesis procedure. Furthermore, they are expected to show a better performance as blend stabilizers since they form broader interphase regions. Further research on operative procedures is needed in order to facilitate the production of these materials and aid in the study of their applications.

The copolymerization of styrene (St) and methyl methacrylate (MMA) has been extensively studied, particularly for the production of block copolymers. Gradient St-MMA copolymers would be interesting for improving applications where their block counterparts are currently used. The reactivity ratios of St and MMA are similar and less than unity, so that both comonomers favor cross-propagation. For this reason a spontaneous one-pot polymerization leads to an alternating structure. In consequence the only way to prepare gradient copolymers of St and MMA is through an appropriate feeding policy of comonomers. Several different gradient profiles could be desirable, such as linear, hyperbolic, or blocky gradient, which may lead to different final properties. Manufacturing a material for a pre-specified application requires a precise knowledge of the formed structure. However, the majority of the reported experimental policies for synthesizing these copolymers has been developed by trial and error, something that makes it very difficult to achieve a precise gradient profile. In this context, comprehensive mathematical models are valuable tools to determine the produced molecular architecture and find optimal operating policies to obtain tailor-made materials.

In this work, we present a mathematical model able to predict both average properties and the full bivariate MWD of gradient copolymers of St and MMA mediated by TEMPO. The most common experimental strategies used to produce these copolymers are analyzed with the aid of this model. Typical experimental policies reported in the literature are simulated in order to determine the exact composition profile that results from them. In addition, optimal policies necessary to produce different specific gradients are obtained. The model is a valuable tool in the design of novel materials with pre-specified characteristics.

[513]

Degeneracy Hunter: An Algorithm for Determining Irreducible Sets of Degenerate Constraints in Mathematical Programs

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Degenerate constraints, i.e. constraints that violate the Linearly Independent Constraint Qualification (LICQ), are prevalent in many chemical engineering applications including flowsheet optimization problems, both due to poor model formulations (typically human error) and features such as recycle loops. Furthermore, they are very problematic when solving nonlinear programs (NLPs), resulting in a singular matrix being inverted during a simple Newton step. As a result, most modern solvers implement counter-measures to detect and eliminate degenerate threats. We have observed these methods require noticeable computational effort and don't always work. The best approach is to reformulate the original NLP. Unfortunately, this is difficult for complex models with thousands of equations.

Degeneracy Hunter is an algorithm that systematically analyzes any iteration from a continuous mathematical program solver and determines irreducible sets of degenerate constraints. This allows the expert modeler to focus on only a handful of equations, instead of the thousands that may be in a large problem. There are four key steps in Degeneracy Hunter algorithm:

1. Import first order KKT information (Jacobian, multipliers, etc.) and determine the active set based on Lagrange multipliers. Restrict the search set to strongly active, active or all inequality constraints and/or bounds based on user specified settings.
2. Factorize the Jacobian of the constraints and identify non-pivot equations. These are candidate degenerate equations.
3. For each candidate degenerate equation, solve a mixed integer linear program (MILP) to identify an irreducible set of degenerate equations containing the candidate equation. The MILP essentially calculates one singular vector while minimizing the total number of equations in the irreducible set (equations with non-zero entries in the singular vector).
4. Report the names of equations and the singular vector for each irreducible set.

The Degeneracy Hunter algorithm has been prototyped in MATLAB and analyzes KKT information exported from GAMS. The MILPs at the heart of Degeneracy Hunter is also solved in GAMS. The algorithm has been tested on a variety of large, non-convex NLPs, including an Air Separation Unit (ASU) design problem with 15,000+ variables and constraints [1]. Using Degeneracy Hunter, three different types of degenerate equations were identified in this particular ASU problem. Straightforward revisions of the model to remove these degenerate constraints resulted in a 16% decrease in average computational time. Identifying these degeneracies would have been virtually impossible without a systematic approach.

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[517]

Optimization of gas detector placement for real-time prediction of accidental release incidents

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The release of hazardous materials in chemical industries can be detected by gas detectors network. In this paper the proposed technique of determining the optimal placement of gas detectors focuses on the "detection" of all possible release events. Using dispersion models for the simulation of all possible release scenarios and specific optimization package to solve the mixed-integer programming problem, different objective functions are calculated, for example, the minimum number of detectors required, the minimum expected time to detect release scenarios with fixed number of detectors. Though gas detectors are primarily used for detecting the release, they could do more. Authors' previous study on the real-time prediction of release event using gas detectors, dispersion models and artificial neural networks has proposed an alternative approach for the prediction of the distribution of release gases in emergency response. The new approach could bypass the requirement of sources terms that are essential for dispersion models and use a small group of gas detectors along with neural networks to build the inner-connections between the causes (source terms) and consequences (gas dispersion). In that approach, one group of gas detectors could only cover limited range of wind directions for real-time prediction of release events with single source. The purpose of the present paper is to find the optimal placement of gas detectors, covering all possible scenarios including all possible weather conditions, process conditions and multi-sources, to implement the real-time prediction of all possible release events in emergency response. A developed mixed-integer linear programming problem is presented for determining the optimal placement of gas detectors, considering the cooperation between neighbor detectors. PHAST, a widely used commercial consequence analysis tool, is used to generate thousands of scenarios with various leak locations and weather conditions. Three objective formulations are explored: minimize the expected detection time with variable scenario coverage constraint (which determines the proportion of scenarios that are applicable to the real-time prediction technique), minimize the expected prediction time while maximizing the scenario coverage, minimize the expected prediction time and number of detectors used with fixed scenario coverage. The extensive MILP problems are solved using CPLEX. In all examples, the cooperation of gas detectors is considered and the minimum number of group detectors that could effectively predict the two-dimensional dispersion of released gases is applied. Results show that the scenario coverage constraint significantly affects the number of gas detectors needed. Furthermore, and it has been demonstrated that the prediction-purposed, optimization-based gas detector placement technique is applicable for the real-time prediction of accidental release incidents.

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Dynamic Multi-Objective Optimization of Batch Chromatographic Separation Processes

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Optimal isolation of a high purity target component from a multicomponent mixture is of significant importance in the pharmaceutical and biochemical industries. The complexity of the fermentation broth from the production of recombinant proteins calls for sophisticated purification methods. One of the most widely used and most successful purification methods in this area is preparative chromatography. However, the removal of closely related product impurities, both in terms of size and charge, are usually challenging even for high resolution (analytical) chromatography separation with high performance resins and optimized elution mode. Likewise, the determination of two essential fractionation or cut-times with reproducible selectivity is critical.

Solvent composition gradient elution is widely applied in both analytical and preparative chromatography. Studies on gradient elution operation are exclusively devoted to quantify and optimize step gradients, linear gradients or more sophisticated nonlinear (concave and convex) gradients with respect to various performance indices (e.g. quality and cost of separation). However, a generalized optimization framework for off-line trajectory planning of liquid chromatographic separation processes in batch elution mode has not been developed. Therefore, the main purpose of the present study was to demonstrate a generally applicable model-based methodology for simultaneous optimization of elution trajectories, target component pooling decisions, and column loading factor. The realistic multi-component system dynamics required for analysis were generated by numerical solution of the reaction-dispersive model, governed by a set mass-balance partial differential equations (PDEs), with a modified Langmuir isotherm and experimentally validated kinetics. Hence, the proposed methodology implies formulating and solving a large-scale dynamic optimization problem (DOP) constrained by PDEs. However, in chromatographic separation processes, there are several incommensurable objectives (e.g. production rate, yield and product pool concentration), which require a trade-off to ensure a satisfactory design. For the purpose of this study, a set of Pareto solutions are generated for bi-objective (production rate and yield) scenarios by means of a weighted metric method. Thus, this method combines multiple objectives into a single performance index.

This contribution describes the realization of a new off-line dynamic optimization methodology for batch chromatographic processes. The developed model is encoded in the Modelica language and a simultaneous optimization method, based on collocation on finite elements, is applied using the optimization extension Optimica and the framework of JModelica.org. The DOP is thus translated into a nonlinear program (NLP), which is very large. To efficiently solve the NLP, derivatives together with sparsity patterns needed for the numerical optimization solver are computed using algorithmic differentiation. The potential of the general dynamic optimization (open-loop optimal control) framework is illustrated through the solution of a specific challenging ternary complex mixture separation problem, with the intermediately eluting component as the target, by hydrophobic interaction chromatography (HIC). A key result is the Pareto optimal solution set, which successfully reveals the relation between the incommensurable objectives and provides a qualitative framework to evaluate the optimal solutions.

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An Adaptive Multi-Objective Differential Evolution Algorithm for Solving Chemical Dynamic Optimization Problems

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Dynamic optimization problems appear frequently in many different industries and the solution of dynamic optimization problems is extremely important for better performance of process industries. However, these problems are quite challenging because they often involve multiple and conflicting objectives. Multi-objective evolutionary algorithms are effective to solve multi-objective dynamic optimization problems (MDOPs), because they can yield a set of Pareto optimal control variables in a single run. In this paper, an adaptive multi-objective differential evolution (MODE) algorithm named EPSMODE is presented to solve the MDOPs using the control vector parameterization approach. Firstly, by approximating the control variables with piecewise constant functions, the original MDOP is transformed into a static multi-objective optimization problem with several undetermined control parameters. Then, EPSMODE is proposed to optimize these undetermined parameters. In EPSMDOE, an ensemble of control parameters and mutation strategies are employed, and compete to produce offspring based on Pareto domination mechanisms. Employing the ensemble technology can choose appropriate control parameters and mutation strategies during different stages of the MODE evolution for a specific MDOP, and generate Pareto optimal fronts with better convergence and diversity. Its application to three MDOPs, compared with other state-of-the-art MODE algorithms, reveal the effectiveness of the proposed approach.

[590]

Optimal operation of a pyrolysis reactor

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Recently, the worldwide olefins production (mainly ethylene) increases rapidly (approximates 180 billion lb/yr), and is regarded one of the most significant issues for chemical industries where improving its production operation can bring several benefits. Thus, the market demand for olefins production has accelerated the improvement of a more rigorous and reliable thermal cracking model of such process. Its annual industrial production depends on the thermal cracking (pyrolysis) of oil hydrocarbons, where the heart of the process with a massive economic effect is the reactor of the cracking process. Cracking of heavier fuel oils is done to produce mainly high quality (octane number) petrol, olefins (feed for petrochemical industry), coke (by coking) and to reduce the viscosity of fuel oil (by visbreaking)(1-3). The main parameter of the optimal design of such reactor is the accurate prediction of yield and reactor performance. Each reactant is known to produce a certain distribution of products. When multiple reactants are employed, it is desirable to optimize the amounts of each reactant so that the products satisfy flow and demand constraints. Control systems are designed for achieving several goals, involving product quality, safety, and minimum cost. Many operations can be employed in olefins production in spite of the process, which is favored in modern practice includes the cracking reactions (2,4).

In the present study, the problem of optimization of thermal cracker (pyrolysis) operation is discussed. The main objective in thermal cracker optimization is the estimation of the optimal flow rates of different feeds (such as, Gas-oil, Propane, Ethane & Debutanized natural gasoline) to the cracking furnace under the restriction on ethylene and propylene production. Thousands of combinations of feeds are possible. Hence the optimization needs an efficient strategy in searching for the global minimum. The optimization problem consists of maximizing the economic profit subject to a number of equality and inequality constraints.

Modeling, simulation and optimal operation via optimization of the thermal cracking reactor has been carried out by gPROMS software. The optimization problem is posed as a Non-Linear Programming problem and is solved using a Successive Quadratic Programming (SQP) method (which is regarded to be one of the most promising approaches for solving constrained nonlinear optimization problem in addition to its successful application to many engineering optimization problems with high accuracy(5)) within gPROMS (general PROcess Modelling System) software.

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[600]

Representation of the Convex Envelope of Bilinear Terms in a Reformulation Framework for Global Optimization

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Branch-and-bound type algorithms in combination with convex underestimators are often utilised in global optimisation of nonconvex mixed-integer nonlinear programming (MINLP) problems. Another option is to rely on reformulation-based techniques such as the αSGO (α signomial global optimisation) algorithm. In αSGO method power and exponential transformations for signomial or polynomial function as well as the α-reformulation technique for general nonconvex twice-differentiable functions are used for reformulating the nonconvex problem. The resulting problem is a convex reformulation of the original one in an extended variable-space, and the global solution is then found by iteratively solving and refining the obtained problem.

In a branch-and-bound algorithm, it is possible to use different convex underestimators in different subdomains (represented by a node in the tree) of the problem. In a reformulation framework however, this is more difficult; therefore bilinear terms have until now been regarded as signomial terms in the αSGO algorithm and no specific transformation strategy have been used, even though the convex envelope, i.e., the tightest underestimator, is known. This has resulted in a less tight convex underestimation of bilinear terms compared to, e.g., branching-based methods. For any solution method tight convex underestimators are essential, so therefore a reformulation strategy for bilinear terms resulting in the convex envelope is given in this paper. The strategy can be applied to pure bilinear problems or, in combination with the other transformation strategies of the αSGO algorithm, to any nonconvex MINLP problem containing bilinear terms.

[611]

Interactive Multi-Objective Decision-Support for the Optimization of Nonlinear Dynamic (Bio)Chemical Processes with Uncertainty

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The manufacturing industry is faced with the challenge to constantly improve its processes, e.g., due to lower profit margins, more strict environmental policies and increased societal awareness. These three aspects are considered as the pillars of sustainable development and typically give rise to multiple and conflicting objectives. In this respect, the EU growth strategy Europe-2020 confirmed this trend by indicating sustainable development as the only way to operate in industry and the Global Report Initiative [1] identified more than 100 Key Performance Indicators (KPIs) for evaluating sustainable development.

Dynamic mathematical models and model based optimization techniques have for more than 30 years contributed to improvements in economic sustainability (e.g., maximize profit or production) of industrial processes [3]. However, much less effort has been spent on: (i) the inclusion of societal and environmental impact within optimization studies, (ii) the quantification of the impacts and trade-offs arising between them, (iii) the proposition of different optimal improvement alternatives and (iv) the making of well-informed decisions for the operation of industrial processes under uncertainty. Typically, a single solution that optimizes all conflicting objectives simultaneously is not possible, but there exists a set of mathematically equivalent solutions, known as the Pareto set [2]. To support decision making in practice multi-objective optimization can be exploited to help the decision-maker generating different Pareto optimal alternatives and choosing among them.

Hence, any decision made will require trade-offs to be evaluated and compromises to be made. To support decision making an interactive multi-objective framework is presented to optimize dynamic bio(chemical) processes based on mathematical models. The framework is not only able to deal with multiple objectives but it also includes a numerically efficient strategy to account for parametric uncertainty in the models. Consequently, optimized solutions that are robust in view of constraint violations can be obtained and objectives related to the operational risk can be accounted for. The introduced interactive framework for multi-objective dynamic optimization under uncertainty is successfully tested for a five-objective chemical reactor case study with uncertain parameters.

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Superstructure Optimisation of a Water Minimisation Network with an Embedded Multi-Contaminant Electrodialysis Model

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The water-energy nexus considers the relationship between water and energy resources. With the increase of environmental regulations in the process industry with regards to both these resources, it is desirable to develop techniques that minimize the amount of freshwater used and wastewater generated from process operations, while simultaneously minimizing energy and capital costs required to do so. Conventional water network optimisation is often performed using superstructure optimisation, wherein many simplifying assumptions are applied to regeneration units to describe their performance, such as fixed recoveries and linear cost functions. This approach, commonly referred to as the "black box" approach, does not consider energy consumption and therefore provides an inaccurate representation of costs and limits the practicality of the model.

This work proposes a mechanistic superstructure optimisation approach that contains a detailed energy-minimization regeneration model. The regeneration unit considered is a multi-contaminant electrodialysis unit. The model takes into account a set of fixed and variable parameters essential to the design and operation of an electrodialysis unit. It is imbedded in a water network that comprises several water sources and sinks. The superstructure promotes water minimization as it allows for the possibility of direct recycle and reuse as well as regeneration recycle and reuse. The overall model contains continuous, integer and binary variables, and is nonlinear, rendering it a mixed integer nonlinear program (MINLP). The model is solved to minimise a cost function that takes into account operating and investment costs of retrofitting a regeneration unit. The developed model was applied to a pulp and paper case study, where it resulted in a 20% savings in freshwater consumption and a 26% decrease in wastewater production. The overall cost of the water network (freshwater, wastewater treatment, piping interconnections and regeneration cost) decreased by 23%. This was achieved while simultaneously determining the optimum operating and design conditions (e.g. area, current, pressure drop) of the electrodialysis unit required to minimise energy requirement.

[620]

Deterministic Global Optimization and Transition States

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Transition states (index-1 saddle points) play a crucial role in determining rates of chemical transformations but their reliable identification remains challenging in many applications. In the current literature deterministic global optimization methods have been employed for the location of transition states (TSs) by initially locating all stationary points and then identifying the TSs among the set of solutions [1,2]. The drawback of this approach is that computational time is spent for the location of "uninteresting" solutions (i.e. minima, maxima and higher-order saddle points). Aiming to focus the computational effort on the location of TSs of general nonlinear functions (twice-continuously differentiable), we introduce regional tests for the identification of hyper-rectangular areas that do not contain any TS or that may contain a unique TS. These tests, applied to the interval Hessian, are based on the interval extensions of theorems from linear algebra. They can be used within the framework of global optimization methods with the potential of reducing the computational time for TS location. We present the theory behind the tests and results on simple benchmark functions.

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A Metaheuristic for Solving Large-Scale Two-Stage Stochastic Mixed 0-1 Programs with the Time Stochastic Dominance Risk Averse Strategy

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Supply chains are complex networks of entities and flows that recently have evolved to consider closed loop systems where forward and reserve chains are simultaneously considered. Under this extended systems the treatment of uncertainty has been recognized as crucial although the resulting problems, usually large-scale two-stage stochastic problem result in complex system to be solved.

In the present paper we aim to contribute to the solution of this problem. We study general two-stage stochastic mixed 0-1 problems, where the uncertainty appears anywhere in the objective function, right and side and constraint matrix coefficients. The 0-1 variables and continuous variables have nonzero coefficients in both stages. A metaheuristic algorithm is proposed as a specialization for two-stage problems of the so named Fix-and-Relax Coordination Algorithm (FRCA) for solving large-scale multiperiod stochastic mixed 0-1 optimization problems. So, in the multiperiod multistage case as in the multiperiod two-stage case the large-scale character can be motivated by the intrinsic dimensions of the problem as well as due to the large number of additional 0-1 and continuous variables and constraints required by the risk averse strategy to use. In this work it is the time consistent stochastic dominance constraint strategy, so-named SDC, as mixture of the first and second-order stochastic dominance constraint risks averse measures induced by mixed-integer linear recourse plus considering a time consistency policy.

A main characteristic of the inexact approach that is proposed consists of considering so-named levels along the time horizon included by disjoint sets of consecutive periods. At each level an independent partial scenario mixed 0-1 model is solved by fixing the 0-1 variables of ancestor levels to the value obtained at the optimization of their related models and relaxing the integrality of the 0-1 variables related to successor levels as well as the (cross scenario SDC systems) for those other levels. Additionally, the continuous variables are obtained at each level by considering the bound targets of the SDC systems up to that level.

In order to assess the solution procedure applicability, computational tests were performed on multi-period and multi-commodity closed loop supply chains randomly generated from a deterministic reference case previously addressed in Salema (2010), that being a large scale case, its stochastic counterpart is a very large one. Computational results are provided.

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[738]

A technology superstructure model for decision making in biorefineries

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One of the major challenges in the design of biorefineries, is the identification of sustainable portfolios of products to match market and process uncertainties, as well as handle multiple feedstocks [1]. Second-generation biorefineries, in particular, are characterized by a plethora of processing paths to treat the biomass, which might lead to complex portfolios of products. In such a complex variety of options, it is crucial that the value derived from biomass feedstock when processed in a biorefinery is maximised [2]. This could happen to the extent that the economic feasibility and environmental sustainability of biobased production systems will be both guaranteed through sustainable product manufacturing and energy generation [3].

The research debate is still open on the way to produce more sustainable biobased products identifying and promoting the most promising technological solutions [2]. The application of process synthesis and design techniques could help boosting this innovation [1].

Technology superstructure models have been applied to handle the complexity of bio-based production systems. Superstructure models consist of synthesis blocks that for given objective functions (e.g. minimisation of cost, minimisation of greenhouse emissions, maximisation of profit, minimisation of energy requirement etc.) could support and steer investments in future biorefineries, choosing among alternative solutions [4]. In fact, these decision support platforms might provide a holistic approach about the available and feasible combination of biomass processing options, and help define optimal strategies according to various criteria (e.g. economic, technical, environmental, social, etc.) [5]. Optimisation tools enable the performance of sensitivity analysis, assess technical or economic uncertainties, and identify the major cost drivers of the examined options [6].

This work will focus on the development of optimisation tools to support strategies for the screening and evaluation of biomass-to-bio-based chemicals production routes. A technology superstructure model based on mixed integer linear programming (MILP) is proposed to generate optimal routes to selected products (e.g. ethanol, xylitol, itaconic acid) obtained from biomass. The methodology will enable a systematic process design to convert biomass into products and the identification of cost centres. Opportunities for process and energy integration will be explored in order to improve the overall system profitability.

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[790]

Unit-specific continuous-time formulation for the scheduling of biopharmaceutical batch and continuous processes

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Scheduling optimization has become an essential aspect in the management of most industrial processes. To be competitive in the current globalized market, companies need to handle large portfolios ensuring flexible manufacturing processes and active responsiveness to demand fluctuations. With the increasing complexity to operate these multipurpose plants, the challenge to provide efficient scheduling tools has motivated the research community for the past years. Several industrial applications of scheduling models and methods have been applied successfully supplying a number of different approaches to fit the wide diversity of optimization problems. Despite the major developments so far, the implementation of such models to large industrial problems often stumbles in either to address specific operational requirements or to tackle large temporal horizon due to inherent computational complexity. The development of efficient modeling techniques able to solve real industrial problems remains an open topic, by exploring formulations to address the constraints of the different processes and aiming the full integration with common decision-making systems.

The case of the pharmaceutical industry is a good example of how market is driving the change on product development and manufacturing activities. The sector is expanding into the development of highly effective bioengineered drug treatments for diseases such as cancer, diabetes or growth disturbances, but presents some limitations in the supply of large scale productions. The manufacturing process of these biopharmaceuticals is characterized by two complex steps: the upstream steps include all tasks associated with cell culture and maintenance, and downstream steps comprise the chemical/physical operations in the isolation and purification of the drug components. The specifications of these biochemical steps have identified optimization problems in the planning and scheduling of biopharmaceutical facilities, such as, long campaign basis to minimize changeovers or cross-product contamination, biological variability of fermentation yields, products storage shelf-life limitations and strict regulatory policies of production lots. Such problems are still an open research issue within these new type of processes.

Regarding the modeling challenge, the general formulation approach based on the unified process representation of a State-Task/Resource-Task Network (STN/RTN) have proven to be effective in most classes of scheduling problems. However, within biopharmaceutical processes such representations have not yet been widely explored.

In this paper, we follow this challenge and present the development of a mixed integer linear programing (MILP) model based on the RTN formulation, using now a unit-specific continuous-time formulation for the scheduling of a multi-stage multi-product process of the biopharmaceutical industry. The model addresses some of the scheduling constrains of these bioprocesses, such as, the sequence of batch and continuous tasks, the storage constrains of products regarding shelf-life limitations, and the track-control of the production lots for regulatory policies. The model is applied to a benchmark problem in the biopharmaceutical industry and the results discussed to related literature.

[797]

Optimized production of multilayered monodisperse polymer nanoparticles.

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Over the last two decades, the nanotechnology has undergone a fascinating resurgence of interest in different disciplines and engineering areas, such as biology, medicine, catalysis, energy, etc. One of the most important and difficult tasks for researchers and engineers in the field of nanotechnology is to produce nanoparticulate materials with perfectly tailored end-use properties at the industrial scale. This requires an effective control of the physical, chemical, and morphological characteristics, such as particle size distribution (PSD), particles morphology, glass transition temperature (Tg), and in the particular case of polymeric nanoparticles: molecular weight distribution (MWD) and polymer microstructure.

Multilayered nanoparticles have drawn particular interest in the area of drug and gene delivery, biosensors and the development of miniaturized optical, electronic, optoelectronic, information-storage materials and devices. Different technics have been used to synthesize this class of nanoparticles, particularly self-assembly and layer-by-layer deposition. In this paper, multilayered polymer nanoparticles are produced through emulsion copolymerization of styrene and butyl acrylate. The main objective is to optimally control the production of predesigned multilayered morphology in a lab scale semi batch reactor. To achieve this goal, the time dependent feed profiles of pre-emulsioned monomers are computed under a multiobjective dynamic optimization framework. Two objective functions are considered: one objective function is inherent the gel transition profile describing the targeted multilayered morphology and the second reflects the maximization of the overall yield. In addition, the optimization problem embeds several constraints including the requirement of a monodisperse size distribution.

The production process entails four main stages. The first stage aims at producing the primary polymer particles under batch conditions. The first layer is produced through the second stage, during which pre-emulsioned monomers are fed separately to the reactor, in order to achieve the designed end-use properties expressed in terms of gel transition temperature profile. This stage ends when a targeted particle size is reached. At this point, the temperature is temporarily raised to consume the residual monomers prior the subsequent stages. The whole procedure is repeated during the next two stages. A large predictive dynamic model of the process has been developed and validated elsewhere. The model turns out to be highly non-linear, non-smooth and hybrid. This makes non-deterministic tools more appropriate and cost effective to address the optimization problem at hand. As such, a genetic algorithm is used to compute the Pareto set of the non-dominated solutions, which provides the different operating trade-offs.

[875]

Systematic Design of Chemical Reactors with Multiple Stages via Multi-Objective Optimization Approach

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Optimal staging of chemical reactor design via multi-objective optimization approach is investigated in this study. The approach consists of the following steps: identifying path-dependent design variables, selecting several (possibly conflicting) design objectives, and solution of the corresponding problem by using multi-objective optimization algorithm. The corresponding approach is investigated for two industrially important reactor systems: ethylene oxide and phthalic anhydride synthesis. By using reference-point based multi-objective evolutionary algorithm (R-NSGA-II), Pareto-optimal solutions are generated within the region of user-specified reference points, thus facilitating the selection of final optimal designs. Apart from the extensive selection of optimal candidate designs, the approach also enables further insights to be obtained regarding the optimal arrangement of path-dependent design variables along the reactor length.

[879]

Synthesis and Design of Integrated Process and Water Networks

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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 considering 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. Since the connection between the process network and the wastewater treatment network is not straight forward connection, a new converter interval is introduced in order to convert into wastewater stream characterization. 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 superstructure-based optimization methodology is shown to be a useful decision support tool for early stage synthesis and design networks by screening a large number of design alternatives for the networks. 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.

[903]

Optimization of High-Density Polyethylene Slurry Process Based on Molecular Weight Distribution and Chemical Composition Distribution under Uncertainty

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High-density polyethylene (HDPE) is widely used as the main material in the film, pipe, and container industries. Currently, introduction of copolymer to the HDPE polymerization process can significantly improve the performance of the product due to the balance of microstructures. Microstructure of copolymers such as molecular weight distribution (MWD) and chemical composition distribution (CCD) are thus of great importance for evaluating quality of HDPE products. However, due to technical restrictions, current measurement methods introduce uncertainty to the microstructure of polymers. Symmetric deviation of the GPC trace leads to a broaden MWD and TREF profile can only provide apparent values of CCD, which of the uncertainties give rise to discrepancy of HDPE product. This work addresses the optimization of HDPE product with expected MWD and CCD under these uncertainties. The formulation of the optimization problem includes uncertainty metric of target MWD and CCD and productivity optimization of the HDPE process. A decomposition strategy is adopted to deal with the uncertainty at upper level and process rigorous model at lower level. Linear Taylor expansion of the target at design point is used to characterize the “worst case” adopting deterministic approach. Then the operation conditions are optimized in the process model. An industrial HDPE slurry process is discussed and the results show a good reduction of uncertainties and give more flexibility to operation conditions.

[928]

A Systematic Approach for Targeting Zero Liquid Discharge in Industrial Parks

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The increasing environmental pressures to minimize wastewater discharge from industrial plants to the environment have led to the emergence of policies and regulations that promote Zero-Liquid Discharge (ZLD) solutions. These systems are typically associated with high capital and operating cost and pose a significant economic burden to implementing industries. ZLD solutions are explored as End-of-Pipe treatment options to eliminate liquid discharges. Instead, ZLD options should be explored in the context of overall water integration of industrial facilities to achieve desired reductions in water footprints through efficient reuse together whilst achieving ZLD.

In this work, we propose a systematic approach to screen sustainable and low cost strategies that will assist in targeting water integration for Zero Liquid Discharge (ZLD) in industrial parks. The approach expands an Eco-Industrial Park (EIP) representation for water integration to include different possible ZLD options. A mixed integer non-linear programming (MINLP) model for water integration in industrial parks is developed to screen the representation. The optimization model represents a decision support tool that can help the designer in quickly evaluate potential reuse and recycle scenarios with ZLD. The model is formulated to allow streams to be reused internally and externally in each plant, recycled in a shared centralized and decentralized treatment and in ZLD systems, and utilized for a number of options that can constitute ZLD including beneficial usage and/or ZLD processing. The default objective is to achieve ZLD at minimum total annual cost.

A case study of an industrial park with three plants has been solved and analyzed in a number of scenarios to illustrate the usefulness of the proposed model.

[938]

Decomposition techniques for the real-time optimization of a propylene production unit

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Real time optimization strategies are used to evaluate and determine the optimal operational conditions of a plant, maximizing the economic productivity of the process subject to operational constraints (Jang et al., 1987). If the optimization problem encompasses the whole refinery, it can be solved by creating a plant model and maximizing profit with respect to the market prices of the plant's inputs and outputs. However, in practice such centralized approach cannot often be effectively applied due to the size and complexity of the problem. One solution is to use decentralized optimization, the optimization problem should be decomposed and solved in divisions, with reduced numerical complexity. Such decomposition, however, requires that division's inputs and outputs must be priced (Jose and Ungar, 1998). A unit of propylene production was modeled in EMSO (Environment for Modeling, Simulation and Optimization) (Soares and Sechi, 2003). The unit was decomposed in three divisions that are the Depropanizer, the Deetanizer and the C3 Splitter.

It is shown that a traditional technique, the so-called "Lagrangian relaxation" outperforms in this example for two main reasons: the process contains some indifferent divisions, which are divisions where there are no linear dependencies between the objective function and the complicating constraints. The second cause is that the divisions objective function are linear, in this case, the active constraint of the optimizations problems will always be the capacity bound of each division and not any intermediate flow (Jose and Ungar, 1988).

One alternative technique called "pricing interprocess streams using slack auctions" was also applied to the process studied. This technique defines slack resources over the process streams and prices them using slack auctions (Rinaldo and Ungar, 2000). It is shown that this technique also fails, because all the divisions have two different products, these means that the technique will always produce the maximum flow of the final product in each division and not any intermediate product.

As those problems in the decomposition techniques were identified, a modification of the Lagrangean relaxation algorithm is proposed. This modification adds one constraint to the second and third divisions. This constraint represents the availability of intermediate product to be processed and is updated at each iteration.

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[955]

An approach to deal with non-convex models in real-time optimization with modifier adaptation

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Real-time optimization (RTO) is a technique that is frequently used to optimize the operation of a plant in real time. RTO uses a model of the process and available measurements to determine the optimal values of the independent variables that lead to the minimization of some cost function. Typically, these optimal values are passed asset-points to the control system with a frequency that is in the order of several minutes or hours. However, due to model errors, such as parametric and structural errors, the RTO solution can lead to an operating point that is different from the real optimum of the plant or not even feasible in practice. To deal with this situation, RTO applications often use some adaptive strategies to update the model with measurements. An example of these strategies is given by the classical two-step approach, which performs two optimization calculations. First, it updates the model parameters by minimizing the error between model predictions and measured values; and second, it performs the minimization of the objective function. To correct structural errors, the experimental determination of the gradients of the objective function and constraints are often included. This seeks to enforce the Karush-Kuhn-Tucker optimality conditions in the real plant when the RTO strategy converges to a local optimum. The technique ISOPE (Integrated System Optimization and Parameter Estimation) adds gradient correction terms to the objective function, while the Modifiers Adaptation technique addresses the active constraints and the objective function. In complex systems, however, the presence of nonlinearities and non-convexities may lead to the existence of multiple local solutions. The gradient corrections of the model, which are implemented by using measurements obtained in close proximity to a local solution, may not be able to identify global changes that can affect the location of the true global optimum. Hence, leading to local optimal solutions, which are not necessarily global solutions. To overcome this drawback we propose a new framework that extends the traditional RTO method by incorporating an upper layer that deals with the global optimization of the more rigorous non-convex model. By doing so, we aim at locating a solution which lies within the region of attraction of the global solution of the actual plant. This solution is then refined by using the modifiers adaptation technique. The implementation of the method is shown in a case study which is related to the optimization of a continuous stirred up tank reactor (CSTR). The CSTR and traditional RTO system are implemented in Matlab while the global optimization layer is implemented in GAMS and connected via a Matlab-GAMS interface. We show how the proposed approach over-performs the RTO technique based on the modifiers adaptation algorithm by leading the system to the true global optimal solution.

[1006]

A robust minimax Semidefinite Programming formulation for optimal design of experiments for model parameterisation

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This paper addresses the model-based optimal design of experiments (MbODE) via Semidefinite Programming (SDP). We consider the continuous representation of the optimal design as a probability measure mathematically described by a two-dimensional tuple containing the sampling points and the fraction of times each one is sampled. This framework allows writing the problem of finding the optimal design of experiments for a particular model as a convex optimization problem. The objective function is a given metric of the Fisher Information Matrix (FIM) assuming that the model errors are independent and normally distributed. There are several ways to minimize the asymptotic confidence region of the parameters, each one leading to different criteria (e.g. the D-optimality minimizes the generalized variance by minimizing the volume of the confidence ellipsoid of the model parameters; and for A-optimality, we minimize the (squared) diagonal of the bounding box of the confidence ellipsoid). When the models are nonlinear the FIM is dependent on the parameters, and one can not derive a closed form for the design, since the confidence region depends on the local value of the parameters. There are three different approaches to handle the circular dependency: i. employing successive local optimal designs arising from model linearization; ii. employing a prior distribution to represent the parameters uncertainty with the optimal design minimizing a Bayesian representation of the FIM; iii. employing a robust formulation to determine the optimal design for the worst efficient parameters' combination. This latest paradigm is used in this paper.

In the later years, SDP formulations to find optimal designs for both linear models and nonlinear models employing the Bayesian framework were derived. Both representations require initially the discretization of the space of regressors into a finite set of points, the construction of local FIM, and the solution of the SDP problem generated weighing local FIM by the fraction of measurements of each point. Here we use a similar procedure to build a robust counterpart (RC) problem corresponding to minimax optimal design in a finite set of alternatives. Each discretization point yields a Linear Matrix Inequality that is enclosed in the RC problem. The FIM is computed from the sensitivity of with respect to parameters. To account for the uncertainty of the parameters we use a Monte-Carlo sampling scheme based on a prior distribution. To avoid the impact of sampling scheme we use a Successive SDP algorithm, which relies on the sequential solution of the SDP problem for a different set of parameter combinations. Therefore, the construction of FIM and the solution of the SDP problem is iterated until a pre-defined tolerance level is met.

Our strategy is demonstrated in a model describing the dynamics of concentration of three species in a CSTR where a sequential reaction occurs. The sensitivity equations are solved together with the dynamics for each parameter combination. The SDP problems are codified using cvx, a Matlab compatible environment that supports a particular approach to convex optimization, before employing SeDuMi, a SDP solver. This solver in turn uses the Interior Point method with a primal-dual predictor-corrector scheme and a self dual embedding.

[1015]

Dynamic Modelling and Optimal Design of the Solid-Phase Reactive Chromatographic Separation System for Biomass Saccharification via Acid Hydrolysis

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Biomass is a renewable and largely available low-cost source of sugars which can be hydrolyzed and fermented to produce bioethanol or converted to other value-added chemicals. The hydrolysis reaction of biomass using strong acid is one of the common processes; however, the main drawbacks are the cost of acid recovery and the sugar degradation with byproduct formation such as hydroxymethylfurfural (HMF) and furfural which not only reduce the sugar yield but also strongly inhibit the subsequent fermentation process to produce bioethanol.

Solid phase reactive separation system (SPRSS) has been proposed in our previous work1 which could potentially improve sugar yield and less byproduct formation from biomass saccharification process via acid hydrolysis. This process integrates the progressing batch reactor (PBR)2 and simulated moving bed chromatography (SMB) where both have similar principles of the switching of all liquid inlet and outlet ports to imitate the solid phase movement. SPRSS could also be applied to other system that involves solid reactants.

This work will present the dynamic modelling and optimization of the SPRSS focusing specifically on the PBR operation. The SMB chromatography model has been developed with numerous operating schemes.3 Nevertheless, the dynamic modelling of the PBR operation is not well-established. While PBR is also a kind of cyclic chemical processes which involve port switching that mimics countercurrent operations, several steps in PBR operations such as emptying and loading the solid biomass requires several unique assumptions on the initial conditions that need to be carefully justified. The optimal PBR design at cyclic steady state will be compared with that from an approximate countercurrent reactor model at steady state.4

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[1050]

Design of a multi-contaminant water allocation network using multi-objective optimization

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Due to the environmental problems, strict policies and regulations concerning the water industrial use and discharge had forced the industry to treat their effluents. During the last decades, the scientific community has been largely involved in the topic of the design of optimal water networks while minimizing both economic and environmental objectives. The core of this study is to design Water Allocation Networks (WAN) defined by a superstructure integrated by different processes, regeneration units and contaminants. The problem formulation is based on mathematical programming and can be either linear or nonlinear according the studied case. A general approach has been proposed in [1] to tackle the problem of the design of optimal water networks. The Mixed Integer Non-Linear Programming (MINLP) embeds all network types considering either mono- or multi- contaminants, thus leading to a generic attractive formulation. The network formulation allows allocating the different streams of the network while minimizing several criteria. The multi-objective problem is solved by ε-constraint and lexicographic methods to obtain the Pareto Front and a Multi-Criteria Aid Decision Making (MCDM) tool based on the so-called M-TOPSIS method (Modified Technique for Order of Preference by Similarity to Ideal Solution) is then selected to choose the best compromise solution. In this work, the optimization framework proposed in [1] is applied with specific focus on large-scale WAN design problems involving multi-contaminants and several regeneration units, that constitutes a major challenge. A case study for a simplified petroleum refinery [2] is treated and analyzed from a multi-objective viewpoint. The problem consists of five water-using processes and three treatment units with three contaminants (i.e. hydrocarbon, hydrogen sulfide, and suspended solids). The literature source underlies the optimization of the total costs (taking into account the regenerated water flowrate). Feng et al. [3], solved this problem by minimizing freshwater consumption, regenerated water flowrate and contaminant regeneration load using sequential optimization to design an economical water network for this system. Their results are compared to those obtained in this study by minimizing three objectives, i.e., fresh water consumption, number of network connections and the regenerated water flowrate using ε-constraint and lexicographic methods to obtain a larger number of potential solutions. The comparison of different solution strategies (i.e. sequential optimization and in this work the ε-constraint method) constitutes the originality of this work. The GAMS environment with Bonmin solver was selected. As a perspective, new constraint could be added to the WAN design problem involving multi-contaminants and several regeneration units to integrate the Heat Exchange Network (HEN).

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[1060]

Optimization studies through simulation of a Methanol/Water/Glycerol Distillation Column

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Many industrial companies struggle to survive in a competitive market and are looking for additional measures to increase processes efficiency. Some companies have been operating for many years with the pre-established conditions provided by the process installer. However, since processes first startup, changes may have occurred which would require a new tuning of the control variables. At the same time, testing different conditions may not be acceptable due to restrict timetables for goal production quantities to be achieved. The growing use of process simulators by research groups has allowed a greater deepening of process knowledge without disturbing the usual operation.

Although some optimization studies for efficiency increase, aimed the complete process, others are focused on large energy-consuming units. The distillation is not only the most used separation process in chemical industry, but also in many cases a major energy consumer achieving a significant percentage of the overall site thermal energy consumption. Creating distillation columns models in process simulators allows performing optimization without disturbing the process, which is a good tool to improve energy efficiency. When considering the economic optimization of a distillation column, this must account with investment costs when considering the type and number of trays as well feed location, and operating costs when considering the desired composition output and several operation conditions. With a reliable model which accounts with economical parameters it is possible to quantify not only the energy consumption of the column but also the total cost for different operating conditions with the objective to achieve optimal design. In already running columns, several optimization variables which are available in design phase are not susceptible to be modified. Some examples are the number and type of stages, feed location, pressure drop along stages which depends of configuration, etc. Others remain available for optimization as reflux ratio, supplied heat in the reboiler and feed stream temperature. Other important aspect when operating columns it's to minimize disturbances of feed stream which may be expressed by temperature or composition variations which may result in a shift of the optimal conditions and a need of new adjustments. Disturbances in utilities streams may also result in additional difficulties in maintaining not only the product purity specifications but as well the optimized conditions.

This work addresses the operating conditions optimization of a distillation column for methanol/water/glycerol separation, for a biodiesel production process with the objective of establishing a better relation between the distillation process variables for a more energy efficient operation. Due to a consumption of 35% of thermal energy of the all process, any minor modifications may have an economic significant impact in the operating costs. A comprehensive Aspen-HYSYS model based on thermodynamic and physical data of the distillation column was developed. The model was validated comparing it output data with available industrial real data. The result was studied for the influence of various design parameters and elements.

[1086]

Simulation and optimization of the ethane cracking process to produce ethylene

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One of the most important processes in the petrochemical industry is the cracking of light hydrocarbons to produce commercially more important products such as light olefins and aromatics, which are considered key components of the chemical industry. This process is carried out at high temperatures in a tubular reactor located in large gas-fired furnaces that supplies heat. The topic of this work is to apply process optimization to the operation of thermal cracking of ethane in order to maximize the production of ethylene. The cracking reactor was modeled as a one-dimensional tubular reactor, and the kinetic mechanism used here is a detailed free-radical schemes that was carefully selected from literature. This application is a challenging problem because of the presence of a free-radical mechanism that coupled with material, energy, and momentum balances of the reactant-product flow along the reactor leads to stiff differential equations that are difficult to solve. In this work, these differential-algebraic equations are discretized using orthogonal collocation on finite elements, and the collocation equations are used as equality constraints in the non-linear optimization problem. GAMS optimization-modeling platform is used to implement this optimization problem. A comparison between model results and experimental data shows that the used approach is a good alternative for dealing with this type of optimization problem.

[1114]

Study of performance of a novel stochastic algorithm based in Boltzmann Distribution (BUMDA) coupled to self-adaptive handling constraints technique to optimize Chemical Engineering process

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The optimal design of distillation systems is a highly non-linear, multivariable and multimodal problem due that the rigorous model of distillation columns is represented by MESH equations and phase equilibrium calculations (Thermodynamic model); also, has several local optimums and subject to several kinds constraints such as, design constraints, topology scheme, and achieve targets of purity and recovery for each component of split. In this paper, we propose employed a novel stochastic algorithm called Boltzmann Univariate Marginal Distribution Algorithm (BUMDA) coupled to self-adaptive handling constraints technique to optimize a well-know distillation process scheme. The problem optimization consist in minimize the total reboiler duty in a distillation train to split a four components mixture. The BUMDA's performance is compared with Differential Evolution (DE) due that this last algorithm is used frequently in optimization of distillation columns. The results show that the BUMDA algorithm is better than DE algorithm regarding effort computing, quality solution, and time to find solution; so that BUMDA algorithm is efficient, trusted, easy use and of general applicability in any chemical engineering process.

This study verifies that the approach presented in this paper, BUMDA algorithm with self-adaptive handling constraints technique, is a powerful and robust tool capable of optimizing processes in chemical engineering and potentially useful in other engineering areas.

The most important conclusion, is that the BUMDA algorithm is better than DE algorithm, because BUMDA is capable of find best design with low numeric effort, short computing time and good success rate, highlighting the fact that the reinitialization mechanism of the variance allowed major exploration on the search space and diversification of the population, reducing the possibility of remaining on local optimal; giving as result best values along of the optimization process.

[1125]

Multi-objective MINLP optimisation of chemical process flowsheets combining rigorous and shortcut models in a novel process synthesis framework

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The study currently underway makes use of a novel framework for the synthesis of optimal flowsheets in order to find optimal process configurations for chemical processes. Designing flowsheets for chemical operations can be a complicated task. Choices in one area of the plant can affect other areas of the plant downstream. Further, there often exists a large array of process options to choose from with differing positive and negative connotations for both the economics of the plant as well as environmental and safety issues. Modern advancements in mathematical programming have allowed for simultaneous flowsheet optimisation, allowing for solutions that have been shown to decrease costs of manufacturing, over traditional sequential and heuristic approaches.

The novel procedure used in this study generates flowsheets in the following way. First a superstructure is generated for the problem in question, by screening potential technologies. This superstructure is then modelled as a mixed-integer non-linear programme (MINLP) making use of "black-box" and approximate models with a number of potential processing options embedded in the superstructure. The selected 'optimal' flowsheet is then simulated rigorously, unit by unit, using a process simulator such as ASPEN or using rigorous simulations to check whether the shortcut models in the MINLP are realistically attainable. With the outputs evaluated, the MINLP is then modified to more accurately reflect the simulated model, providing a more realistic solution in the operating regimes selected by the MINLP model. The optimisation is then re-run and the new flowsheet assessed and simulated. This process is repeated until convergence upon a solution is obtained. In this way it is possible to use both the explicit equation formulations required for rigorous optimisation of process variables, while maintaining a lower level of complexity for the MINLP solution strategy and also ensuring the "black box" models are appropriate for the specific operating regimes selected.

If a particular unit formulation in an MINLP run is not able to be accurately simulated, then large corrections have to be made and these corrections are potentially only applicable to certain unit operating regimes. This can lead to the exclusion of this process option from further iterations. In order to deal with such cases, a limit is applied to the amount of correction that can be applied per iteration.

While the methodology cannot guarantee global optimality, it can ensure that the synthesised processes are physically achievable, a drawback of some other studies, and has also been shown to converge on physically meaningful parameters without the explicit formulation of complicated non-linear equations in the MINLP formulation. Another benefit of the newly developed approach is that the insights obtained during the detailed simulation and MINLP optimisation steps, are used to further refine the MINLP superstructure, so as to guide the solution to an optimal point not only based on economics, but based on environmental impact as well.The novel solution strategy is applied to a variety of processes, including heat exchanger network design, the hydroalkylation (HDA) process and a bioethanol plant, all with solutions that are comparable with other widely published synthesis techniques. The new procedure can also find application in the synthesis of other processes.

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Track 3. Cyber-Infrastructure, Informatics and Intelligent Systems

[75]

On the Process of Building a Process Systems Engineering Ontology Using a Semi-Automatic Construction Approach

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This work presents a novel systematic approach for the construction of domain ontologies. The suggested approach uses a semi-automatic construction methodology. For this study, parent-child concept pairs are taken from a previous work. Novel contributions include building and completing branches, introducing new relations, and resolving inconsistencies and contradictions. For the process systems engineering (PSE) domain the ISA88 Standard is chosen as a promising starting point for automatic text processing. Finally, this work concludes with a discussion of the ISA88 Standard based on the conclusions that can be obtained from the application of this semi-automatic construction methodology.

[446]

Constructing an ontology for physical-chemical processes

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An ontology is a formal collection of pieces of knowledge that specify the behaviour of entities in a domain. Our domain is physical-chemical-biological systems, processes that we describe with a set of concepts or principles. These ontologies are not used to reason about the system, but to construct process models that adhere to these concepts[, in particular the conservation principles and the behaviour of materials, the geometrical concepts in space and time.

The paper will discuss the systematic construction of an ontology having set the condition that the definition space must be lower triagonal, or in other words context free, or more pictorial like a bootsrap: one starts with a minimal defintion and constructs the rest on top without reaching ahead. So picking it up is a one-pass operation: start at the beginning and pick up one piece at the time building the whole of the building representing the core knowledge that is used to represent physical-chemical-biological system.

The approach has also a very close relation to the system theory's behaviour theory [1][2]. For more references on the subject see also [3].

The objective of the project is to generate a model-centred framework for computational engineering activities in the wider domain of chemical engineering.

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[500]

Graphical Processing Unit (GPU) Accelerated Solution of Multi-Dimensional Population Balances Using High Resolution Finite Volume Algorithm

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Population balance modeling is a widely used approach to describe, crystallisation processes, taking into consideration the primary phenomena as nucleation and growth, as well as particle agglomeration and breakage. The population balance model can be extended to multivariate cases where more internal coordinates i.e. particle properties are used, which can be, for instance, the sizes of crystal faces enabling the description of particle shape. However the particle composition (e.g. in co-crystallization), age and temperature may also be applied as internal particle coordinate. The solution of the generated partial differential equation is not trivial due to its hyperbolic nature which causes numerical dispersion and diffusion during the numerical solution. Gunawan et al. (2004) proposed a high resolution finite volume algorithm (HR-FVM) for multi-dimensional population balance equations, which is based on the idea that using a flux limiter function numerical oscillations can be eliminated and higher integration time steps can be applied. Despite of these advantages of the HR algorithm, the computational time is still significantly larger, compared to e.g. the standard method of moments based solution. A crucial feature in using models in real-time applications is the fast solution (typically at least 1-2 order of magnitude faster than the process). More recently there is in increased interest to apply parallel computing and computations using graphic processor (GPUs), which typically have a hardware architecture consisting of multiple parallel computing units (Wei and Kruis, 2013). The current study presents two accelerating possibilities for HR-FVM. Compiled c/c++ code in form of .mex file is used to accelerate the computation on CPU and compiled CUDA c/c++ code in form of .ptx file handled by the Matlab Parallel Computing Toolbox is used to run the simulation on a GPU. The case studies demonstrate that the HR-FVM run on the GPU was between 5-10 times faster than the compiled c/c++code and 50 times faster than the standard Matlab implementation. This significant improvement in computational time enable the application of model-based control approaches in real time even in the case of multidimensional population balance models.

[563]

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

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Recently, novel modelling environments have been developed in order to support re-use of mathematical models and to allow for combined use of different modelling frameworks in order to study a wide variety of processes, including highly complex processes. Two major issues have motivated the need for an integrated framework solution within the context of (bio)-chemical process modelling. The first issue is that some process models consist of complex subsystems that cannot be modelled and simulated in a single general-purpose tool. The second issue is the need to support model re-use. Also, the computer aided modelling system should offer new capabilities for users to write mathematical models in different formats and/or to provide various options for model transfer. One of the most time consuming challenges for model developers has been exchanging information between computer systems and tools.

The model re-usability is important, since process modelling tools usually have different software implementations; consequently, the models provided by a computer aided modelling tool may only be accessible via a programming interface in a certain language. This problem can be overcome through a computer aided modelling tool that provides a component interface following certain standards, such as, CAPE-OPEN, COM-object, XML or DLL.

In this contribution a general model framework for systematic modelling procedure through modelling templates, which supports both, the derivation of models from scratch, and the reuse and evolutionary modification of an existing model via its import and export model capabilities is presented.

A feature allowing the XML transfer of models within the framework parts and also use of COM-objects to translate information to other applications is highlighted. Moreover, the ICAS modelling framework, allows transfer of models from/to MOSAIC modelling environment, which, in turn, gives a possibility to translate models to the various languages, such as C++, gPROMS®, GAMS, Aspen Custom Modeler® and Matlab®, including a full model documentation. This connection and transfer of models between different tools will allow the use and analysis of models in the most efficient way, depending on the goal of modelling (identification/parameter estimation, process control, parameters estimation, process design, system representation/understanding, etc.). Regarding the model import, the possibility to import mathematical models in a native text file format is available in the ICAS modelling framework. The mathematical model can be created in a text editor program and then saved as a text file. Then the model will be pre-screened and pre-translated to make sure that it is valid. The application of the modelling transfer feature is highlighted with the case study for batch reactor and batch distillation.

[602]

BiOnto: An Ontology for Biomass and Biorefining Technologies

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Ontologies are a very useful tool for knowledge representation. Their potential has been recognised in many different domains such as the biomedical, legal, financial, agricultural and chemical and process engineering (CPE).

In the domain of CPE ontology development efforts have focused on process and process systems design, supply chain modelling and industrial symbiosis and environmental decision-making among other fields. This ever increasing use of ontologies is due to their important role in formalising the diverse and volatile information and concomitant opportunity to analyse and understand the knowledge of a domain and respective sharing and reuse of the domain knowledge.

This paper presents an ontology, the BiOnto intology, which expands on already successfully developed processing technology ontology and represents knowledge about biomass and biorefining technologies. To this end, the BiOnto ontology provides a reference model that is interpretable both by humans and computers by classifying biomass in 5 different ways: i) processing characteristics, ii) chemical composition, iii) physical properties, iv) existing standards, and v) waste-based classification. More specifically, the ontology/classification has been designed in order to be enable use of biomass in a number of scenarios, which include screening of processing technologies for particular type of biomass, screening the alternative technologies to target material or energy output, selecting the best technology to satisfy set economic, environmental and/or social targets, and screening biomass types to supplement already used one. In addition, the BiOnto ontology can be used in applications such as searching and indexing of biomass information, enabling interoperability between applications, data integration and enabling and enhancing decision making in relation to biomass and biomass processing.

BiOnto has been validated within industrial symbiosis applications, but also with the use of a number of scenarios involving biorefineries, their processing technologies and their possible inputs, outputs and performance. It has been proved to support informed decision making taking into account both efficiency and processing options.

[607]

Linking process, electrical and logical connectivity for supported fault diagnosis

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Many engineering activities depend on the proper analysis of the plant topology (structure of the underlying process/system). In particular, process operation requires a thorough understanding of the interconnections between units to be able to evaluate diverse operation scenarios. These interconnections can happen via material, information and electrical flows. The development of Topoviz™ has been based on user studies, a comprehensive study of XML standards for storing plant data, analysis of CAE systems and interviews from several experts in the field.

In the user interface of the proposed tool, where engineers are able to extract relevant information about the pant topology which are hidden metadata from schematics and databases. This is achieved by the use of intelligent parsing algorithms that traverse the data structures looking for connections between instrument and variable tags, using the LINQ to XML methods (Iyun, 2011). The topology data is then integrated into a network using methods from graph theory such as the property-graph model. This network structure is then linked to a user interaction layer where the engineer is able to visualise, perform queries and explore the plant topology. In a typical graph visualisation, highlighting, filtering and zooming can be achieved. Nodes and edges in the graph display detailed information when selected.

The proposed paper reports several advances compared with previous work in Birk et al. (2010), Schleburg et al. (2013), and Yang et al. (2014). These include the generation of a novel graph structure that presents several advantages over adjacency matrices, signed digraphs and other object oriented modelling methods. Furthermore, the algorithms extract connectivity information from electrical diagrams as well as from the process P&IDs. The step of linking electrical equipment with process diagrams in plant topology analysis has never been achieved before. It greatly enhances the capabilities of the analysis, for instance when causes of disturbance originate or are propagated through the electrical system.

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[621]

An interactive framework for building and analysing models of urban energy systems

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This paper describes a software framework for building and analysing models of urban energy systems. The framework consists of a technology database and components for model assembly and networking coupled with a graphical user interface. The technology database, which is implemented as a Protégé ontology, describes the available energy conversion, storage and transportation processes. The spatial framework for the model is defined by a cityspace object. The distribution of demands, resource flows across infrastructure networks, and the location of energy conversion processes are specified within this cityspace. The user interface instantiates and assembles framework objects into an overall object model of the system. The assembled object model can be used to define optimisation scenarios for the design of urban energy systems with specific goals and constraints such as minimising investment costs while meeting emission targets. These scenarios can be submitted across a network to a solver on a remote host to obtain an optimal design of the urban energy system. The results are displayed by the user interface at two levels: an aggregate level with key performance indicators and graphical analysis for the city as a whole, and a detailed level showing information about individual cells and flows between cells. The interface also provides charts and summaries for comparing alternative scenarios with variations in emission targets, cost parameters and available technologies.

[650]

Natural Language Paradigms for the Model-based Analysis of Waste Management Systems

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Waste Management Systems are complex interactive networks of data, knowledge, models that take into account and process multiple parameters. In these systems the technologies along with their models interact with each other in order to fully describe the problem. Inputs and outputs of the models intersect depending on the various parameters. The parameters need to be computed simultaneously (such as composition, pH, temperature etc) in order to select the appropriate processing path prior to model development. Therefore, the context of the models is adjusted by the path selected and the waste stream characteristics. The need to synthesize the multidisciplinary domains of waste, integrate the knowledge and express them with common natural language terms is outlined by this work.

The work builds on recent technology that was produced to synthesize superstructures for integrated biorefineries (Magioglou et al. 2014) [1], which now extends to decision-making and allocation problems for waste management systems. The approach employs ontologies [2], Java language [3], OpenBabel library [4] and suggests a natural language framework. The natural language modeling ensures the reusability and promotes sharing. The use of ontologies focuses on the automation of path selection and the extraction of the required data. OpenBabel library contributes in automation of the chemical composition analysis of the waste streams. Java language develops the framework, integrates and coordinates the different parts.

The approach is illustrated for an industrial wastewater treatment system of the chemical sector which evaluates the environmental impacts. The models describing the system calculate life-cycle inventory parameters as a function of the wastewater composition and the technologies applied. The framework successfully synthesizes the network and allocates the waste, technologies, streams, auxiliaries' networks along with their parameters.

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[771]

Enterprise-Wide Scheduling Framework Supported by Knowledge Management

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The short-term scheduling problem consists of organizing the available human and technological resources in the process plant in order to optimally satisfy customer's demands. Scheduling typically involves decisions on the amount of products to be produced, equipment and resources allocation, production sequence and operations timing, on a weekly or daily basis. A significant amount of models have been proposed in the literature in order to adequately formulate scheduling problems (Floudas & Lin, 2004; Harjunkoski, 2014). However, each modeling option is only able to cope with a subset of the features, and the choice of the mathematical model has an important impact on computational performance. As a result, the model selection and corresponding problem formulation is a formidable task. From a descriptive perspective, computer science provides with tools for representing the scheduling problem from an abstract conception. For example, artificial intelligence and semantic models, such as ontologies, offer the alternative to represent and share the knowledge of the process and engineering domains. Ontologies are increasingly seen as a key semantic technology for addressing and mitigating the effects of heterogeneities and for enabling semantics-driven knowledge processing. Ontologies are formal structures enabling acquiring, maintaining, accessing, sharing and reusing information (Fensel, 2003).

The goal of this work is to provide a knowledge-based framework capable of determining the best available mathematical models for specific scheduling requirements based on the problem description. Specifically, this work aims to exploit the knowledge found in Operations Research Ontology, by the integration of a decision application and a mathematical scheduling models database. Hence, models capabilities and limitations must be carefully considered for each scheduling problem based on its features and the expected computational performance. A semantic model has been created based on rigorous analysis of existing process scheduling models. Likewise, a reasoning tool is developed for matching the scheduling problem features to the available mathematical models. As a result, a model selection will be obtained based on features matching.

Several case studies stemming from the scheduling literature illustrate the performance of the framework and present the advantages and limitations of the proposed approach.

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[789]

Knowledge Management Support to the Integration of Scheduling and Supply Chain Planning using Lagrangian Decomposition

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The integration of planning and scheduling decisions in rigorous mathematical models usually results in large-scale problems. These problems are highly complex, since they require substantial level of detail to describe the system appropriately. Among the several approaches to tackle the issue of complexity, decomposition techniques based on duality and information flows between a master and a set of subproblems, such as Lagrangian decomposition, have been widely applied.

Ontological models allow the virtualization of systems and processes and can therefore be easily used to translate such reality into holistic mathematical models, thus facilitating the use of analytic tools and providing higher flexibility for model building in industrial environments. Likewise, ontologies improve information sharing and communication within system entities which is highly relevant for the integration of decision-making and its supporting modeling frameworks Overall, ontologies are a powerful tool for improving the integration of decision-making in industrial environments, where large amount of data are available.

This work aims to exploit ontologies in order to address the optimal integration of planning and scheduling using a Lagrangian decomposition approach. Scheduling/planning sub-problems are created for each facility/supply chain entity and their dual solution information is exchanged by means of the ontological framework, virtualizing the reality. This way the integration of planning and scheduling problems and the corresponding solution strategy are executed seamlessly by employing the ontological framework.

Two case studies based on a STN supply chain planning and scheduling models are presented. The case studies concern a waste treatment complex, where significant cost savings and environmental impact reductions can be gained by optimizing the allocation of different types and amount of wastes. The system of the waste plant consists of the following components: external and internal tanks, different types of waste and different lines of waste process (technologies for waste treatment). The advantages and limitations of the proposed approach are emphasized.

[847]

Towards a Methodology for Reusable Ontology Engineering: Application to the Process Engineering Domain

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Existing methodologies for ontology engineering, focus on the good practice of ontology development. Their main aim is to develop an ontology that is consistent following certain principles and also ensuring that the described domain is complete. To our knowledge none of the existing methodologies focus on developing ontologies that are easy to reuse. In addition to that, methodologies introduced in the domain of Process Engineering adopt a high level approach rather than specific and detailed steps. Although the aim of this work is to propose an ontology engineering methodology that supports reusability of ontologies, the main target of ontology engineering should remain to create ontologies that are useful before being reusable. The proposed methodology is a result of the experience during the eSymbiosis project.

The name of the proposed methodology (MetROn) has been inspired from the ancient Greek proverb "παν μέτρον άριστον", meaning "all in moderation". As in life where extremes are not often the solution, in ontology modelling/engineering there is not a single solution, not a single method and not a single way to develop an ontology. This methodology does not attempt to dictate how a correct ontology is developed but rather how to correctly develop an ontology.

The proposed methodology combines steps from existing methodologies and adds to them from the experience of developing the eSymbiosis ontology. As most of existing methodologies in the literature focus on the theoretical side of ontology engineering, this work attempts to relate each step to the domain of Process Engineering. Besides defining these steps, this paper also provides some helpful guidelines that facilitate the reuse of the developed ontology.

MetROn consists of 8 distinct steps and describes how each one of them affects the reusability potential of the developed ontology. The development process is initiated with the widely established step of defining the domain and the application of the ontology. Step 2 involves the identification of existing ontologies that define the same or similar domains. For the next step the engineer should consider other available resources even if there are not any available ontologies for reuse. Another commonly accepted step is the identification of the terminology of domain, tools and methods for this step are presented. Steps 5 and 6 discuss potential methods for defining the classes and properties of an ontology. Step 7 revisits the consideration of reusing existing ontologies, this time referring to complementary information. The last three steps refer to more practical aspects of ontology development, namely the namespaces, restrictions and annotations of the ontology and how they affect the reusability potential of the ontology.

This methodology is a result of the development of the eSymbiosis ontology, an ontology that has been successfully employed in a web platform that supports and automates Industrial Symbiosis practice. MetROn has been verified through the development of the eSymbiosis ontology. In order to objectively validate the methodology, it has also been verified through the development of another ontology representing knowledge about biomass and biorefining technologies. The results of the development process are also presented.

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[1093]

An ontological approach to integration of planning and scheduling activities in batch process industries

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Nowadays, the importance of effective tools for supporting planning and scheduling activities in the batch process industries is undeniable. Despite over twenty years of research in batch scheduling, advanced scheduling support systems are not very common in the chemical industry yet. In addition, almost all commercial systems that are available nowadays are not based on the many solution methodologies that academia has developed. One of the most important reasons why academic approaches are not adopted in industry is the fact that planning and scheduling decision support tools do not integrate with the enterprise and manufacturing applications that are regularly used in industrial organizations. In fact, the planning and scheduling activities need to be addressed within the context of the enterprise hierarchical planning pyramid. This pyramid, which includes activities that are performed at different time frames and handle information having distinct granularities, involves scheduling interplaying with the Production Planning and Control (PPC), as well as with Plant Control (PC) functions.

This contribution addresses the previous integration challenge by proposing a planning and scheduling domain ontology, devised to tackle integration issues. This paper describes the adopted ontological engineering approach; i.e. not only the ontology itself is presented, but also its development process is briefly discussed, starting from the motivation for its construction, the competency questions that defined the scope of the ontology, going then through the conceptualization and implementation stages, and finishing with some validation issues.

Since ontologies are, by definition, based on consensual knowledge, both the ISA-88 and ISA-95 standards, which are well accepted in the industrial domain, have been taken into account during the ontology development. The mail goal of ISA-88 is the control of the batch process, whereas the final goal of the ISA-95 standard is the exchange of information between levels 4 and 3 of its hierarchical model. Though both have a close relationship with the scheduling activity, they differ in terms of their purpose and terminology. According to the ISA-95 standard, the scheduling functions that are of interest (i.e. determination of production schedule, raw material requirements identification, determination of end-products packing and sales schedules) interface to the manufacturing operations and control system ones through product definition information, production capability information, production schedule, and production performance information. A detailed analysis of this standard shows some overlapping with the information and activities handled by the ISA-88 one (e.g. product definition vs. recipe specification, equipment capability vs. physical model, etc.), which indicates some possible collision points. This issue, which has raised some concern among the standard developers has been carefully considered during the ontology development process, and is also addressed in this contribution.

Track 4. Process and Product Synthesis-Design

[24]

Effective Design of Reactive Distillation Columns with Two Reactive Sections

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Reactive distillation columns with two reactive sections (RDC-TRS) in the top and bottom were proposed recently for the separations of quaternary reacting mixtures with the most unfavorable ranking of relative volatilities (i.e., reactants are the lightest and heaviest and products the intermediate). Although feeding the heaviest and lightest reactants to the condenser and reboiler might favor the reaction operation involved, it could pose a detrimental effect to the separation operation involved because the unconverted reactants tended to go through the stage for withdrawing the intermediate product and accumulate at the other ends of the RDC-TRS. For the suppression of the drawback, feed splitting should be adopted in the design of the RDC-TRS (The resultant process design is termed RDC-TRSFS), namely, it is particularly advantageous to feed the lightest and/or heaviest reactants at the top and bottom simultaneously and the splitting ratios can affect greatly the steady-state performance of the RDC-TRSFS. Three examples, including an ideal quaternary exothermic reaction, the esterification of latic acid with methanol, and the esterification of palmitic acid with isopropanol, are employed to evaluate the RDC-TRSFS proposed. Thorough comparisons are made with the RDC-TRS and reactive distillation column with a top-bottom external recycle (RDC-TBER). The RDC-TRSFS is found to be considerably superior to the RDC-TRS and exhibit better or at least comparable performance than the RDC-TBER. These outcomes indicate that feed splitting could serve as an effective means to enhance internal mass integration and internal energy integration in the RDC-TRSFS. Despite that adverse internal energy integration is unavoidable in case of reactions with thermal effect, the RDC-TRSFS could still be considered as a competitive option for the separations of reacting mixtures with the most unfavorable ranking of relative volatilities.

[26]

Improved Design Strategies for Flexible Hydrogen Networks

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Hydrogen integration is a research issue that has recently attracted considerable attention in the petroleum refining industries for operating cost reduction and air pollution abatement. Although several mathematical programming models have already been developed to configure the optimal hydrogen distribution schemes, e.g., see Hallale and Liu (2001), Van Den Heever and Grossmann (2003), Kumar et al. (2010) and Chiang and Chang (2014), there is still room for further improvements. In particular, the deficiencies in current modeling practices can be primarily attributed to (1) illogical unit models and (2) incomprehensive design considerations. A number of corresponding enhancements in deign strategeis have thus be introduced in this work and they are summarized below:

- The hydrogen users (such as the hydrotreaters and hydrocrackers) are traditionally modeled according to fixed throughputs and also constant feed and product concentrations. On the basis of the more reasonable assumptions proposed in this study, not only the inlet and outlet flow rates and concentrations of these units can be treated as decision variables but also their interactions characterized with rigorous material-balance constraints. In addiiton, since the steam reforming plant is often utilized as the primary hydrogen producer in a refinery and, in the existing model, it is simply treated as a source, the more detailed models of its embedded units (e.g., the hydro-desulfurization unit and the PSA unit) have been established and added to the improved mathematical programs. As a result of the aforementional modifications, better design options can often be identified.
- To circumvent the latter drawback mentioned above, the often-encountered seasonal variations in model parameters, e.g., the raw-material costs, the electricity price, the maximum throughput and the minimum allowable hydrogen concentration at the inlet of each hydrogen consumer, etc., have all been incorporated in a multi-period programming model. Furthermore, the decisions to add extra compressors, purifiers and fuel cells can also be quantitatively evaluated by introducing binary variables into this proposed formulation.

As an alternative to the above multi-period model, a systematic timesharing algorithms has also been developed to integrate the conventional single-period designs in different time intervals so as to form a less economical but more flexible network structure for operations in multiple periods. Finally, extensive case studies have been carried out to demonstrate and compare the feasibility and benefits of the two design strategies suggested in this work.

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[36]

An Integrated Reactive Distillation Process for Biodiesel Production

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An integrated reactive distillation process for the production of biodiesel is proposed. The reactive separation process consists of two coupled reactive distillation columns considering the kinetically controlled reactions of esterification of the fatty acids (FFAs) and the trans-esterification of the tri-di and mono glycerides with methanol, respectively. The conceptual design of each reactive distillation column was performed through the construction of reactive residue curve maps in terms of elements. The design of the esterification reactive distillation column consisted of one reactive zone loaded with a solid catalyst (titanium oxide supported on silica TiO2/SiO2) and for the trans-esterification reactive column two reactive zones loaded with solid catalyst (hydrotalcites (CHT) and MgO). Intensive simulation of the integrated reactive process including the complex kinetic expressions for the different reactions and the Cubic-Plus Association (CPA) thermodynamic model was performed using the computational environment of ASPEN Plus. Results showed that the amount of fatty acids (FFAs) and water in the oil fed play a key role on the performance of the trans-esterification reactive distillation column while for the esterification column is not significant.

[76]

A Sequential Algorithm for the Rigorous Design of Thermally Coupled Distillation Sequences

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Thermally Coupled Distillation (TCD) has acquired a renewed interest because, when compared to conventional systems, it is possible to reach over 30% in energy reduction. Besides, if the search space includes Divided Wall Columns (DWC) important investment savings can also be achieved.

One of the major difficulties in the synthesis involving TCD is that the number of alternatives grows up much faster than when only conventional columns are considered. i.e. for a 5 component mixture there are 203 basic configurations [1,2] if we consider also the internal structure of heat exchangers there are more than 104, and if we consider the thermodynamically equivalent configurations the number of alternatives is greater than $2 \cdot 10^5$ [1, 3].

In this work we propose a sequential algorithm, that combines shortcut models (based on FUG methods) and rigorous process simulators to the rigorous design of complex TCD sequences:

Search in the space of basic configurations augmented with internal structure of heat exchangers. Instead of getting just a single solution we augment the search to alternative basic configurations. Divides Wall Columns are explicitly included in this stage. Except for DWC, a task instead a columns approach is used.

A rigorous simulation of the most promising alternatives is performed in Aspen-Hysys to validate the shortcut model or refine the parameters from stage 1 if necessary.

A detailed sensitivity analysis of the internal structure of heat exchangers in order to determine which one could be eventually removed and which of them have an important impact on the sequence performance.

Study of the Thermodynamically Equivalent Configurations to determine 'actual' alternatives, here flow correctors (i.e. pumps around) and possibility of remove some 'transfer blocks' [4,5] are considered.

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[86]

Discovery of New Zeolites for H2S Removal through Multi-scale Systems Engineering

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H2S is a toxic gas found in many chemical and industrial plants, including natural gas processing and utilization, power plants, coal gasification, refineries, petrochemical processing, wastewater treatment, and semiconductor manufacturing. The presence of H2S in natural gas leads to pipeline corrosion during natural gas transportation. Furthermore, H2S is one of the major air pollutants found in tail gases and flues gases from chemical and power plants. Removal of H2S from industrial gas streams with high CO2 and H2S concentrations has become increasingly important due to stringent environmental regulations in recent times. Several technologies are available for H2S removal, which include absorption, adsorption, Claus conversion, catalytic oxidation, catalytic membrane contactor, and microbial treatment.

Microporous adsorbents such as zeolites have been shown to be excellent candidates for molecular gas separation for CO2 capture and natural gas purification. In this work, we apply a multi-scale systems engineering framework to select the most feasible and cost-effective zeolites for pressure swing adsorption (PSA)-based H2S separation from acid gas (CO2/H2S), tail gas, and flue gas mixtures. The key component of this approach is an efficient and hierarchical computational screening that combines discovery of zeolitic materials with advanced modeling and optimization of PSA processes. The in silico screening first exploits efficient algorithms based on geometric and atomistic calculations to screen a database of candidate zeolites and identify those feasible and economical for use in a PSA process. Several material screening metrics are calculated, including shape, size, and pore selectivities. Then, adsorption selectivity for suitable zeolites is evaluated. Zeolites that remain after filtering are subject to detailed mathematical modeling and optimization of the PSA process to calculate the minimal cost, which represents the final ranking criterion. An efficient algorithm based on reduced modeling of the original PSA model using Kriging is implemented to optimize the PSA process conditions while satisfying minimum purity and recovery constraints of 95% and 98%, respectively. The objective is to minimize the combined annualized investment, operating and materials costs of H2S sepration. Using the novel multi-scale computational framework, several new and cost-effective zeolites have been identified for H2S removal.

[94]

Optimization of a Fusel Oil Separation System Using a Dividing Wall Column

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Fusel oil is a byproduct obtained from ethanoldistilleries, composed of a mixture of higher alcohols such as isoamyl alcohol,isobutanol and others. In countries where large quantities of ethanol areproduced alternatives for the use of these byproducts are of great importanceto make ethanol production less polluting and more profitable. As mentionedbefore, fusel oil is a mixture of several alcohols, which limits its direct useas a solvent. The higher alcohols present in fusel oil are considered naturalproducts with high commercial values. For instance, the isoamyl alcohol is themain component of fusel oil, and it can be used in the production of organicesters which are used as industrial solvents, flavoring agents andplasticizers. Fusel oil cannot be discarded directly into the environment,since it would cause undesirable environmental impacts. It is possible somedirect applications of fusel oil: it can be burned to supply energy in thedistilleries or it can be added to diesel fuel to improve the cetane index.Considering the amount of fusel oil in Colombia,a plant capable of producingisoamyl alcohol from fusel oil obtained from different distilleries is aninteresting industrial application since this alcohol is highly valued; itsmarket price is approximately three times the price of ethanol fuel. Due to thepresence of water in fusel oil, heterogeneous azeotropes can be formed betweenwater and most of the higher alcohols. This study aimed to evaluate theindustrial distillation process of fusel oil to obtain isoamyl alcohol,considering fusel oil as a mixture of 9 components. Fusel oil samples,collected in a Colombian industry, were analyzed in order to study the phaseequilibrium (Vapor-Liquid Equilibrium (VLE) and Liquid-Liquid Equilibrium(LLE)). Two configurations for the fusel oil separation process were proposed:the conventional distillation scheme and a configuration using a dividing wallcolumn (DWC). In this study, we have implemented an optimization approach toobtain the design and optimization of two distillation arrangements. Thestochastic method used is a hybrid strategy obtained from differentialevolution (DE) and tabu search (TS). The best design with minimum total annualcost (TAC) resulted in a high recovery of isoamyl alcohol. The results presentedin this work for optimal configuration provide support for development forfusel oil industrial purification plants to obtain the isoamyl alcohol.

[95]

Silane Production through Reactive Distillation with Intermediate Condensers

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The realization that fossil fuels are notinexhaustible and that enhancing recovery of coal, oil and natural gas presentsadditional risks, drives energy policy to scenarios that are based on renewableforms of energy. In most of the proposed scenarios, solar energy is the primaryconstituent as it is the major energy source over large regions. Photovoltaicsuse semiconductor materials to generate electricity from solar energy. Asemiconductor is a solid, mostly crystalline, material such as silicon,selenium or germanium. Semiconductors have electrical conductivities greaterthan insulators but lower than metals which are good conductors. At lowtemperatures they are insulators but at high temperatures and/or when excitedby sunlight, they conduct electrons. The most commonly used semiconductorelement is silicon. Therefore silicon, the starting material for thecrystalline wafer, is the most important material in solar photovoltaics (PV) industry today. To widely commercializethe solar technology, one challenge faced by the PV industry is to decrease themanufacturing costs, especially the cost of solar-grade Si feedstock material.Currently, the most well-known chemical route to produce solar-grade silicon isthe modified Siemens process, which performs decomposition of trichlorosilaneby chemical vapor deposition. This work presents a reactive distillation columnfor the catalytic disproportionation of trichlorosilane to silane whichincludes three consecutive reversible reactions. This reaction system ishowever characterized by a large distinction in the boiling points of the components,which makes the reactive distillation extremely favored. This work shows showthat it is feasible to obtain a high purity of silane over 99% and a completeconversion of trichlorosilane to silane by a typical reactive distillationcolumn. Nevertheless, the normal reactive distillation column possesses theshortage of high refrigeration requirement. By removing heat at temperaturehigher than that at the condenser it is possible to reduce cooling requirementsat the condenser. In this work, a superstructure representation, rigoroussimulations, and optimization problems were combined to derive optimal reactivedistillation columns which can realize heat integration between stages andutilities. An iterative simulation-optimization procedure was proposed toconsider temperature changes in stages due to heat integration. The resultsshowed that the installation of two intercondensers results in the best optionwith economic savings up to 56%.

[99]

Optimal production of Furfural and DMF from algae and switchgrass

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Sugars are an interesting building block not only for the production of biofuels, but also for added-value chemicals. In the biomass typically we can find pentoses and hexoses. While glucose can be used to produce hydroxy methyl furfural (HMF) and dimethylfuran (DMF), xylose can be used to obtain furfural by dehydration. Several papers have presented processes that from different sugars, evaluate these production processes, [1,2]. However, there is not further consideration on the stage that evaluates the sugars production out of biomass which affects the composition of the synthetic mixture, for instance water content, and determines the investment and production costs.

In this work we conceptually design integrated optimal processes for the production of DMF and furfural from two types of biomass, switchgrass and algae. The use of switchgrass allows producing pentoses and hexoses and thus, DMF and furfural can be produced simultaneously. The superestructures are as follows. Switchgrass is pretreated using dilute acid or ammonia fibre explosion. Next, the cellulose and hemicelluloses are hydrolyzed to sugars that are subsequently dehydrated to HMF and furfural. Finally, the HMF is used to produce DMF. In case of using algae, we can produce biodiesel out of the oil, and DMF out of the starch. The algae are grown. The oil extracted and transesterified with ethanol to produce biodiesel. The starch is cooked to produce glucose that is dehydrated to HMF. Finally, DMF is produced from HMF. Simultaneous optimization and heat integration is performed for each process that are formulated as MINLP when we use switchgrass and NLP for the alage based process respectively.

For switchgrass, the use of AFEX pretreatment is recommended for a production of cost of DMF and furfural of $3/kg ($570MM of investment cost). In case of using algae, we obtain 98 MMgal/yr of biofuels, 16% of DMF, at the cost of $1.98/gal ($693 MM of investment). If the sugar concentration in the dehydration reactor increases we can reduce the production costs by 25% and the investment cost up to 50% the base case ones.

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[112]

CO2 as feedstock: a new pathway to syngas

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This contribution presents a pioneering route to synthesize syngas (CO/H2) from hydrogen sulfide (H2S) and carbon dioxide (CO2).

H2S in acid gases and flue gases rich in CO2 represent an environmental issue and an industrial cost as neither H2S nor CO2 is presently used as a major industrial feedstock or commodity. Acid gases mainly come from desulphurization of fossil fuels, and they cannot be simply released, due to their toxicity. H2S is then usually neutralized by conversion to elemental sulfur, with a minor industrial use. Flue gases are massively produced in power, petrochemical and manufacturing plants and CO2, final combustion product, is generally vented to atmosphere. CO2 capture and sequestration is still object of a relevant debate and environmental concern.

By the new chemical route, potential value of H2S and CO2 will be brought out by means of a radically new conversion process: H2S will be thermally activated in a high temperature reactor and will reduce the CO2 to produce H2 via a complex chemical mechanism. Preliminary reactor and process design, along with identification of relevant equipment and operating conditions, led to initial very promising results, which successfully brought to a priority patent [1]. A detailed kinetic scheme, extensively validated in a broad range of oxidation and combustion of sulfur components [2], further supports this oxy-reduction process, marginally observed also in the Claus process.

The paper will be based on four key steps: (1) tuning of the detailed kinetic scheme; (2) identification of the optimal operating conditions and conceptual process design of the high temperature reactor; (3) feasibility study of an industrial plant; and (4) potential applications.

Complete recycle of H2S, relevant reduction of CO2, and additional syngas production from these pollutants represent the valuable environmental, energetic and commercial benefits of the new route, which could also involve a wider field of industrial applications.

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[167]

Design and Optimization of Intensified Non-sharp Distillation Configurations

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According to the U.S. Department of Energy (2012), there are more than 40,000 distillation columns only in North America, and they consume about 40% of the total energy used to operate plants in the refining and bulk chemical industries. Research on process synthesis can find new distillation systems that potentially contribute to save resources and protect the environment. Traditionally, distillation configurations use only sharp split in order to reduce the number of columns and heat exchangers; however, these systems prensent intrinsic thermodynamic inefficiencies, thus one way to reduce these is by means of non-sharp splits. It was demonstrated by Petlyuk et al. [1] that, for ternary non-sharp sequences, the equipment can be reduced by combining the individual columns and by introducing thermal couplings. Moreover, it is shown that employing non-sharp separations can lead to savings with respect to sharp-split configurations [2]. For four or more component mixtures, synthesis of distillation configurations is traditionally based on sequencing simple columns. A simple column performs a sharp or a nonsharp split of a mixture with a condenser and a reboiler. For an N-component mixture, a separation sequence with only sharp splits needs the minimum number of N-1 simple columns with 2(N-1) heat exchangers to achieve N pure products. As the number of columns and heat exchangers are the dominant criteria to evaluate a distillation configuration, traditional distillation configurations with only sharp splits have been the preferred alternatives. In an earlier work, we have presented a systematic method to reduce the number of columns for sharp distillation configruations of quaternary mixtures [3]. In this work, the non-sharp distillation sequence for the separation of a four component mixture is considered, where the non-sharp sequence refers to the possibility of obtaining the product in more than one stream. Using the aforementioned method, different search sub-spaces of alternative sequences were designed by the rigorous equilibrium-stage simulator Aspen PlusV8.0, optimized for minimizing the total annual cost, and the stochastic optimizer Differential Evolution coded in Visual Basic, to finally compared the sequences. The novelty of this work is to show that, starting with this kind of non-sharp configruations it is possible to generate arrangements going from 4 to 3 and to 2 columns, with saving in the energy consumption, space and number of equipments. Moreover, the synthesis methodology used allows to identify two types of intensified sequences according to the type of intermediate column section generated, driving to configurations with less column sections or with divinding wall columns. A method has been developed for both design and optimization of such intensified distillation configurations.

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Deterministic Global Optimization of Multistage Melt Crystallization Processes in Hydroformylation

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Separation of closely boiling mixtures is a challenging problem in process synthesis and process design. A typical example is the separation of mixtures of isomers like n/iso-aldehyde mixtures arising from hydroformylation from renewable resources [1]. Standard distillation is often not favorable due to high process costs. A more efficient separation process for such closely boiling mixtures may be obtained by using melt crystallization either in combination with distillation or as a stand-alone process [1]. To achieve the desired crystal purity, often a multi-stage melt crystallization process is required. Standard approaches focus on countercurrent crystallizer cascades. However, due to restricted process topology this process configuration tends to be suboptimal. Hence, in the present contribution restrictions on process topology are relaxed also allowing new process configurations which have not been studied so far by other researchers to the best of our knowledge. Optimal operating conditions and optimal process structures are determined simultaneously using mixed integer nonlinear (MINLP) optimization. Due to nonconvexity, standard MINLP solution procedures based on local or stochastic optimization algorithms can not guarantee to find the global optimum, which however is essential for identifying also new and probably counterintuitive solutions. Therefore deterministic global optimization using BARON/GAMS [3] is applied. A suitable model of a multistage melt crystallization process for the separation of an isomeric mixture of n-dodecanal and 2-methylundecanal by [1,2] is used. The model is adapted to allow arbitrary process topologies and the resulting model complexity is reduced by reformulating the model equations and excluding redundant crystallizer network configurations. The influence of important model parameters on the performance of new process structures is studied systematically and compared to the standard countercurrent cascade process.

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Design and Economic Evaluation of Alternatives to Effluents Treatment on Biodiesel Production from Soybean Oil and Palm Oil

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Biodiesel production was simulated from crude soybean oil and crude palm oil at industrial level. To better represent the components, real compositions were assumed and some thermodynamic properties were estimated by the method of Constantinou and Gani. It was demonstrated that some changes in the entering streams of the process and in the equipments are needed to reach a fuel in agreement with the international quality laws from the two different vegetable oils, but a same plant could process both. Then, some alternatives to the treatment of the effluents were proposed, including hydrous or anhydrous ethanol production or recycle, pure glycerol production and recycle and unreacted oil recycle. An economic evaluation was performed to find out the better alternative and to compare the potential of both the oilseeds.

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Synthesis of transcritical ORC-integrated heat exchanger networks for waste heat recovery

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This article aims to present a mathematical model for synthesizing a heat exchanger network (HEN) incorporated with a transcritical organic Rankine cycle (tORC) for minimizing the external utilities as well as for maximizing the recovery of waste heat from the heat surplus zone. A tORC-involved stagewise superstructure is proposed for modeling this problem, which has considered all possible matches of heat exchange between process hot/cold streams as well as the organic working fluid. On the basis of this tORC-integrated superstructure, the problem of synthesizing the HEN for minimizing the use of external utilities and also maximizing the recovery of low-grade waste heat is formulated as a mixed-integer nonlinear program (MINLP). A two-step solution procedure is then proposed to solve the MINLP model. A stand-alone HEN is synthesized at first to minimize the external utility. A tORC is then incorporated into the heat surplus zone of the HEN for maximizing the net power from the recovery of waste heat. A literature example is used to demonstrate the proposed model. The performance of the proposed tORC will also be compared with the traditional subcritical ORC by using a lot of examples.

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Efficiency Comparison of Different Design Schemes of Reactive Distillation Process for Ethyl Lactate Production from Fermentation-Derived Magnesium Lactate

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Ethyl lactate is an acid ester widely used as a solvent in several industries. Due to its biodegradability and low toxicity, this ester can be considered as a green solvent. In an attempt to intensify a process for ethyl lactate production, reactive distillation process using magnesium lactate obtained directly from a fermentation as a starting material was designed and simulated in this study. A process flow sheet consists of a reactive distillation column for esterification between ethanol and lactic acid from lactate salt, and a series of fractional distillation columns for purification of ethyl lactate, which was received as an aqueous solution at the end of the process. Process optimization was performed using Aspen Plus simulator equipped with RADFRAC module. Sulfuric acid was used as a homogeneous catalyst, and all the kinetic parameters of the esterification reaction were experimentally determined. Efficiency of two process schemes was explored. In the first scheme, Process A, ethyl lactate was emitted from the top of the reactive distillation column along with other light compounds in the process, i.e. water and ethanol. In Process B, on the other hand, ethyl lactate was discharged from the bottom of the reactive distillation column. The bottom product stream in this process consisted of unreacted lactic acid, sulfuric acid and magnesium sulfate, which were considered as heavy components. Configurations of each operating unit as well as the optimal process conditions were obtained. Process efficiency in terms of overall yield of ethyl lactate, its production rate and its concentration in the final product solution were investigated and compared. The overall yield and ethyl lactate production rate in process A were found to be 93.30% and 273.72 g/hr, respectively, which were much higher than the 73.33% yield and 183.10 g/hr production rate in Process B. However, the final product from Process B was the aqueous solution of ethyl lactate with a concentration of 76.79% by mass, more than twice higher than of the 37.18% solution obtained from Process A. In addition, only 2 fractional distillation columns were required in Process B while 3 were required in Process A to completely purify ethyl lactate solution. This led to the energy consumption in Process B of 71.02 kJ/g, which was much lower than 112.39 kJ/g in Process A.

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Tailor-Made Green Diesel Blends Design using a Decomposition-Based Computer-Aided Approach

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Tailor-made green diesel blend is one of the most promising solutions to reduce the environmental impact while retaining or even improving the performance of diesel fuel. One of the major concerns related to green diesel blends are how to define the blend target properties and how to find blends that match these targets. A systematic computer aided approach can efficiently address these issues and provide a more efficient solution method instead of the iterative trial and error approach. The computer aided technique is able to rapidly narrow down the search space of feasible green diesel blends so that the costly and time consuming experimental works can be done only on the select promising candidates.

This paper will get the optimum solutions of tailor-made green diesel blends by incorporate experimental work together with the decomposition-based computer-aided blend design algorithm. The green diesel blend design problem is solved in three stages. The first stage is to generate blend candidate and study the compatibility of each blend with respect to their stability and compatibility. The second stage is to generate the feasible green diesel blends that match the specified target properties (the design constraints), such as, density; kinematic viscosity; cetane number, higher heating value and flash point. In order to simplify the algorithm, the stage two is decomposed into two sub-steps: (1) match the linear property constraints (density; kinematic viscosity; cetane number, higher heating value) by linear programming model; and (2) further refine the search space by matching the non-linear property constraints (flash point). Subsequently, an optional additive identification step is applied to enhance the blend. At the last stage, the short listed green diesel blends, ranked according to a desired performance index is evaluated experimentally.

This study serves to establish the concept of combining the conventional experimental approach with systematic computer-aided model based approach to obtain tailor-made green diesel blends. The algorithm presented here does not solely depend on the model based approach; it employs a verification by experiment step. That is, employs the expensive and time consuming resources only when necessary for validation.

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Optimal magnesium and calcium precipitation from saline water

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An optimization model is presented for the precipitation of calcium and magnesium from water with high content of these species, such as brackish water, seawater and hyper saline water. The model optimizes the costs associated with the precipitating agents, such as sodium carbonate, sodium hydroxide or calcium oxide. Restrictions include thermodynamic models of precipitation of calcium and magnesium salts, speciation of the species present in the water and mass balances.

Seawater and other saline water are being currently used in flotation process to concentrate copper, gold and molybdenum from ores. However, there are difficulties associated with the precipitation of calcium and magnesium salts, such as low molybdenum recovery and high lime consumption in the flotation of copper sulfides. On the other hand, salt crystallization, such as calcium carbonate and calcium sulfate, is one of the major fouling phenomena encountered in seawater desalination. In desalination based in multi-stage flash distillation technology, the economies are closely linked with heat transfers efficiency, which can be reduced by foulants. In reverse osmosis membranes, fouling has negative consequences such as membrane cleaning, limited recoveries and short lifetimes of membranes. Therefore, the removal of calcium and magnesium ions can improve the desalination and flotation processes.

The results obtained by the model are compared to experimental values. Laboratory tests were carried out with three alternative reagents (Na2CO3, NaOH, and CaO) and their mixtures. The reactants concentration were of 0.025 until 0.1 moles added per liter of dissolution, the maximum removal values of Ca and Mg were 99.6% and 99.9%, respectively. The local samples of seawater from Antofagasta city (San Jorge Bay) were employed. The model showed that it is a suitable tool to optimize the precipitation of calcium and magnesium, either as a pretreatment step in desalination plants or to produce saline water free of magnesium and calcium for mining use.

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Simultaneous Targeting and Process Scheduling with Automated Targeting Model for Batch Water Networks

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Batch processes have recently gained good attention from both industrial and academic sectors, mainly due to the growing trend towards product-centred manufacturing globally. In recent years, many systematic design techniques have been developed for batch processes. Concurrently, the development of various process integration tools for resource conservation has become well established. One of the established techniques for batch water network synthesis is known as the automated targeting model (ATM), where the optimisation formulation is based on pinch analysis to enable flow targeting to be performed prior to detailed network design. One of the advantages of the ATM is its linearity, for which global optimality is guaranteed. Furthermore, it is more flexible than conventional pinch techniques being able to allow cost considerations. In this work, the ATM is embedded in a scheduling framework based on the state sequence network (SSN) representation. The latter has proved to require fewer binary variables compared to formulations based on other representation, and is likely to give better computational efficiency. The inclusion of the SSN formulation enables flow/cost targeting and process scheduling to be performed simultaneously, and the true minimum flow/cost targets to be located. A case study is used to illustrate the proposed approach.

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A Mathematical Programming Targeting Method to Select Treatment Technologies Ahead of Design

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The chemical industry is facing an increasingly stringent legislative framework on discharge limits, while fresh water resources are rapidly depleting. On the other hand industries are struggling to operate in the most economic way. The waste treatment cost depends on the selection of the appropriate technologies and the flowrates of the treated effluents. Prior to detailed designs it is useful to have an overall picture of the maximum potential of a wastewater treatment configuration in terms of the selection of processes to integrate and the minimum wastewater treatment flowrate [1]. Graphical targeting methods [2] are unable to deal with the selection of the most appropriate treatment technologies among alternative options and the production of targets for multiple treatment units. Furthermore, shortcut models for the selection of treatment processes are absent from literature [3,4]. The present work proposes an extension of the transhipment models of Nikolakopoulos et al. [5] in selecting treatment processes besides targeting the minimum treatment flowrates. LP cascade models are transformed into MILP formulations, where integer variables and constraints are introduced to account for the decisions on process selection. The advantage of the proposed method is that it assesses types and capacities of treatment processes simultaneously, further ensuring that any process configuration within the approved set of design features will satisfy the feasibility of constraints. Problems are modelled as transhipment models that act complementary to the water reuse targeting methods proposed by Nikolakopoulos et al. [5], the integrated water targeting and network design approach and the mathematical model of the Total Site approach introduced by Koufolioulos et al. [6] for assisting the optimal synthesis of biorefinery processing paths. The proposed approach addresses targeting problems for treatment systems with fixed outlet concentration or removal ratio. It adopts the concept of concentration interval diagrams proposed for mass exchange networks [7], the transshipment logistics model adjusted to heat exchange network design [8] and the shifting of concentrations procedure proposed for the case of multiple contaminants [9]. Concentrations where residuals of contaminants in these cascade models obtain nonzero values define the pinch point(s) that indicate disconnected design regions and reduce the set of process synthesis variables. The methodology has been tested successfully on problems of systems with various treatment technology and contaminant features.

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Optimal Structure Synthesis of Ternary Distillation System

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A procedure which solves process synthesis and design problems simultaneously is proposed for ternary distillation processes. Heretofore, various process structures such as Petlyuk column and thermally coupled column structures have been proposed for energy conservation of distillation systems, and optimal design procedures have been proposed for each of those process structures. However, even if the number of stages and the reflux ratio are optimized for the direct sequence structure, the structure of Petlyuk column is not generated. In this research, we propose a synthesis procedure in which the process structure and the column design are optimized simultaneously under the superstructure based model. In the proposed synthesis procedure, the composition space of ternary mixture is discretized, and each of the discretized compositions is assigned to a module corresponding to a tray in a distillation column. Then, the superstructure consisting of these modules, which includes all possible vapor and liquid flow routes among modules, is constructed. As the liquid composition of each module is given in advance, all of the constraints can be expressed by linear equations even if the vapor-liquid equilibrium is expressed by a complicated function. Finally, by solving the problem formulated as a mixed integer linear programming problem, the optimal process structure and design condition can be derived. As the composition is discretized, the optimization result includes unessential flows among modules in order to satisfy the material and energy balance at the modules. In the proposed synthesis procedure, by prohibiting the ineffective mixing at each module, such unessential flows are effectively removed. The developed synthesis procedure was applied to several separation problems of ternary mixture. The results showed that the process structure close to the Petlyuk column is created without assigning any process structure in advance.

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Optimization and Analysis of Chemical Synthesis Routes for the Production of Biofuels

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In this work we extend a recently proposed method to concurrently select biofuel blends which satisfy ASTM standards and their optimal synthesis routes by using thermochemistry based post-processing analysis to compare these routes. Gas phase thermochemistry, estimated from group additivity, was used to calculate the ideal gas equilibrium extent of reaction for each synthesis step. Situations of reaction, phase, and site coupling were subsequently identified to overcome equilibrium limited steps and reduce the number of reaction systems required. We posit that this method can aid process designers in screening and ranking large numbers of potential biofuel candidates and synthesis routes simultaneously from an energetic, thermochemical, economic, or kinetic standpoint.

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Design and Economic Evaluation of Coal to Synthetic Natural Gas (SNG) Process

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Natural gas is an important energy source in Taiwan, with increasing demand year by year. It also has recently been considered to be cleaner than other energy sources, due to its lower C/H ratio. However, over 99% of energy source in Taiwan depend on importation, and the requirement of liquefying and pressurizing during transportation make the importation price of natural gas high. Among those energy sources, coal has good advantages over others, including lower price, great abundance, and easier transportation. These reasons lead to the fact that coal is the most used energy source in Taiwan. Thus, a route that converts coal into Synthetic Natural Gas (SNG) is expected to be attractive economically. SNG is a product that holds very similar composition and heat value to typical natural gas, and can be used as a replacement in industries.

The overall Coal-to-SNG process is divided into several parts, including coal preparation, cryogenic Air Separation Unit (ASU), gasification section, syngas treating section (sour water-gas-shift-reaction, syngas cooling, and acid gas removal), methanation reaction section, and electricity production block from upstream to downstream. In the coal preparation step, coal and water form a slurry, and is sent to gasifier with the high purity oxygen (99 mol%) produced from ASU. Gasifier is the core of this process, in which coal is converted to raw syngas through a series of homogeneous and heterogeneous reactions at very high temperature and pressure. Before sending to downstream uses, the raw syngas from gasifier is cooled by Radiant Syngas Cooler (RSC) and water quench, and is then passes through a scrubber to remove ammonia, chlorides and solid particulates. After these steps, the cooled, scrubbed syngas is then entered the syngas treating section. The H2/CO ratio in syngas is adjusted to 3.5 in sour water-gas-shift-reactor, and it is cooled to the required temperature for Acid Gas Removal (AGR). In AGR, dual-staged selexol process is used to capture the acid gases (H2S and CO2), with the capture efficiency assumed to be 99.7% for H2S and 92% for CO2. In the final section of methanation reaction, CO and H2 is nearly completely reacted to form methane, which is the major component in SNG. The heat integration and waste heat recovery in/between different parts are also studied to produce electricity for using inside the Coal-to-SNG plant.

In this work, the steady state design and economic evaluation for Coal-to-SNG process is studied. The overall efficiency for energy conversion is calculated to be at 60.3%; for energy that transferred from coal to SNG, it is at 58.7%. From economic analysis, the overall cost to produce SNG is calculated to be at 11.433 (USD/MMBTU), which is much lower than the price to import liquefied natural gas in Taiwan. Thus, developing a Coal-to-SNG plant will have practically and economically advantages in the near future.

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Water networks synthesis for industrial parks involving inter-plant allocation

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Nowadays, the shortage and pollution of water have become serious barriers to the development of human society. To this end, how to transform the utilization pattern of water from the extensive form of wasting and polluting to the intensive form of saving and cleaning turns to be a key issue facing the process industries. As a promising way of planning for individual plants, industrial parks can provide more opportunities for resources saving and sharing, as well as the centralized treatment of waste. So exploring the reusing possibility in industrial parks, especially investigating the allocation, using and regeneration by breaking process or plant boundary limits would be very meaningful for the global saving and pollution reduction of water in process industries. In this study, we address the challenge to manage the synthesis by regarding the interactions and reallocation (including regeneration) design of water between plants.

Direct and indirect are two ways for water network synthesis when having the inter-plant water allocation problem considered. Therein, the direct reuse is carried out directly via cross-plant pipelines, while the indirect kind must go through the centralized utility hubs (like shared regenerators, water mains et al.) of plants. For the direct kind, it would generate a complicated inter-plant water network if defining the inter-plant water reuse on base of every single unit. To handle this problem, the first part of the study proposes a new direct reuse manner for inter-plant water, by taking the every single plant as basic entity. Such is able to make the all water resources been involved in the all simultaneously ocation even if there is upper limit to the number of inter-plant streams. Moreover, the synthesis complexity of the water networks locating among plants can also be mitigated compared with that on basis of single device.

The second part of the study is to design the overall networks by considering direct and indirect integration. Based on the proposed inter-plant water reuse manner, multiple cases of streams' going in and out a plant are investigated and contrastively analyzed in order to do an appropriate decision-making for the planning. To carry out this work, superstructures representing the possible alternatives with respect to the topologies of water networks are built and formulated with mixing integer non-liner programming mathematical models at different design cases. During the optimization, the fresh water consumption and the inter-plant water flow rate are simultaneously minimized with a two-stage solving procedure. Thus that, it is possible to figure out the internal relations of inter-plant stream number, network structure, fresh water consumption, as well as the collection and redistribution mapping of water among individual plants.

At last of the study, two examples are investigated to verify the proposed approach. Therein, the first example is especially examined to show the application of the new direct reuse manner of water from plants to plants. During the both synthesis, numbers of network alternatives are investigated for the desired solutions in terms of specifying the in and out stream numbers of each plant. With the obtained results, the effectiveness of the approach is demonstrated as expected.

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Sustainable CO2 Conversion using a Process Synthesis-Intensification Framework

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Carbon dioxide (CO2) is one of the main greenhouse gases and therefore methods by which the emission of CO2 can be minimized or utilized are needed. In terms of CO2 utilization, one can explore process routes where CO2 is used to produce value-added chemicals for example methanol and propylene carbonate, among others. The objective of process synthesis is to find the best flowsheet among numerous alternatives for converting specific raw materials to specific desired products subject to predefined performance criteria [1]. In generating flowsheet alternatives that utilize CO2 the unit operations concept, which has been sufficient until now, is one of the most used because it allows the association with tasks that must be performed. However due to the changing chemical industry where, new and more sustainable process alternatives must be designed, having improvements not only in economic but also sustainability/LCA factors, extensions of the current concepts of process synthesis are necessary. An approach to achieving this is by performing process synthesis and process intensification (PI) together where the current search space of unit-operations is extended to include well-known, intensified/hybrid and novel unit operations. A major benefit of such an approach is that truly innovative solutions can be found.

A multi-scale computer-aided framework that performs process synthesis-intensification together and uses the knowledge of the existing methods at different scales, that is the unit operations scale, task scale [2] and phenomena scale [1], has been developed. First, a base case design is found or generated. Second, the base case design is analysed in terms of economics, sustainability and LCA factors in order to identify the process hot-spots. Hot-spots are identified process limitations associated with performing specific tasks. Therefore, minimization/removal of hot-spots leads to the generation of better flowsheet alternatives. These hot-spots are then used to set the design targets for retrofit and/or new design. Third, process synthesis-intensification is performed at the phenomena scale to determine flowsheet alternatives that match the design targets. It consists of combining phenomena (which can be multiple) that perform tasks, which are then translated into unit operations and then flowsheet alternatives. In this way, truly predictive and innovative solutions are generated in the same manner as the combination of atoms to form molecules with desired target properties. Fourth, for selecting the most sustainable design, an objective function that has terms related to economics, sustainability and/or LCA factors is used. Therefore, the best intensified flowsheet which is also a more sustainable option is found.

The paper will present a computer-aided flowsheet synthesis-intensification framework applied to the utilization of CO2 for value-added chemicals. It will be shown that CO2 can be used for the production of raw materials needed for a given chemical process, thereby reducing the net CO2 generation of the overall process where products are produced, CO2 is utilized and raw materials are also produced.

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Robust design of optimal solvents for chemical reactions - a combined experimental and computer-aided strategy

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A new computer-aided methodology for the design of solvents for chemical reactions, recently proposed by the authors (Zhou et al. AIChE J., 2014, accepted), is enhanced and extended. Kinetic models are built by correlating experimentally determined reaction rate constants in a set of solvents with the corresponding solvent theoretical descriptors. The solvent molecular structures are optimized through the formulation and solution of a computer-aided molecular design (CAMD) problem where the descriptors are determined from group contribution methods. Besides the deterministic optimization, a robust solvent design framework is proposed. A sensitivity analysis is performed to assess the impact of parameter uncertainties on the kinetic model. Based on the Monte Carlo sampling of estimated parameter probability density distributions, robust optimization is performed to find solvents promising the best average performance. The proposed methodology is exemplified for a simple substitution reaction and a competitive Diels-Alder reaction. For the substitution reaction, optimal solvents are selected to maximize the reaction rate, and for the competitive reaction, desirable solvents are identified which enhance the formation of the main product while suppressing the formation of the byproduct.

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Energy-saving design and control of a hybrid extraction/distillation system for the separation of pyridine and water

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Design and control of a heterogeneous azeotropic distillation system for the separation of pyridine and water have been studied in Wu and Chien (2009). A two-column heterogeneous azeotropic column system was devised making use of the new minimum-boiling azeotrope between toluene and water. A further intensified dividing-wall column for the same separation system was recently proposed by Wu, et al. (2014) to thermally-couple the two columns for further reduction of the overall reboiler duty. However, from residue curve maps and material balance lines of this system, potential economical pitfall of this heterogeneous azeotropic distillation processes can be predicted due to large recirculation rate inside the system.

In this study, design and control of a hybrid extraction/distillation system for this same separation are studied. Pyridine is extracted from aqueous solution by using N-propyl formate as a solvent in a countercurrent extraction column. Combining two strippers with the extraction column, a simple hybrid extraction/distillation process can be devised achieving the same product purity specifications as the original design.

By comparing the optimized design of this newly proposed system with the previously mentioned heterogeneous azeotropic design, significant reductions of 58.8% in the total annual cost and 65.6% in the steam cost can be obtained. Furthermore, in comparison with the complex design of dividing-wall system, this proposed hybrid extraction/distillation system can still significantly save total annual cost and steam cost by 41.2% and 50.8%, respectively.

The dynamic control of this hybrid extraction/distillation system is also investigated. Dynamic simulations of the proposed control strategy under feed flow rate and feed composition disturbances are conducted in this study. The two product specifications are all well-maintained despite feed flow rate and composition disturbances. Only tray-temperature control was used in the proposed control strategy.

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Alternative Hybrid Liquid-Liquid and Distillation Sequences for the Biobutanol Separation

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The production of butanol throught anaerobic bacteria fermentation of starchy substrates has been reported by Pasteur in 1862. Acetone, butanol and ethanol are the main compounds obtained, the process is usually referred as ABE fermentation, and the butanol produced is called biobutanol. Nowadays butanol is mainly produced as a petro-derived by catalytic hydroformylation of propylene and hydrogenation of the formed aldehydes, this process is known as oxo-synthesis. Since its production is related to the propylene availability, butanol profitability is deeply related to the crude oil price fluctuations. The over consumption of petro-derived products and the necessity to reduce the greenhouse gas emissions, particularly the ones related to the transport sector, has catalyzed the interest in developing bio-derived fuels, like bioethanol and biodiesel. Compare to other biofuels like bioethanol, butanol, has different benefits. It has a higher energy density, it has a lower vapor pressure, it is less corrosive, it is not hygroscopic and it can be blended in any concentration with gasoline or used as a pure fuel without any changing in car's engines [1]. For all these reasons the ABE fermentation process has been reconsidered as a valid alternative to produce bioderived butanol. Among all the process steps, an energy efficient product recovery section is essential for the convenience of the production. It is normally required that the energy used for the butanol separation must be lower than the energy content of the product itself. The present work is focuses on exploring different separation alternatives for the ABE separation proposing new alternatives and a synthesis procedure method that allows the designer to explore a wide set of separation sequences. The new sequences proposed are then compared for their energy consumption and capital costs. As extensively highlighted in the literature, pure distillation processes are proved to be not competitive for this kind of separation [2], but there is still the convenience to combine distillation in hybrid flowsheets with other unit operations. New sequences obtained by the combination of L-L extraction and distillation are obtained introducing thermal couplings and recombining different column section, wich will decrease heat duty impacting directly in total annual cost and it is expected than an environmental indicator it will decrease as same as well. These new sequences were optimized through a global optimization strategy using differential evolution with tabu list as an stochastic method. The alternatives are then compared with the cases reported in the literature obtaining interesting savings in the total annual cost and the environmental indicator.

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Integrated Product and Process Design for the Optimization of Mayonnaise Creaminess

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It has been a long term goal of many fast-moving consumer goods companies to optimize the sensory profile of their products. Fast-moving consumer goods (FMCG) are products which are frequently purchased, consumed on a daily basis, have a low cost-price and are sold in large quantities; for example, foods, drinks, detergents and cosmetics. These products are valued by the consumer on sensory attributes such as: mouth feel, appearance, taste and odor. Via statistical modeling approaches the scores on the sensory attributes were correlated to the physicochemical product properties [1]. The statistical correlations are integrated with product and process models resulting into a modeling framework which enables optimization of the sensory attributes. The philosophy behind this approach is to increase sales by optimizing consumer liking. Therefore the cost function is a mathematical function predicting the sensory score of a particular product attribute as would be given by a tasting panel.

In this context a mayonnaise production line was modeled. Mechanistic and semi-empirical relations were used to model the mixing, i.e. the emulsification process, in particular aiming at the prediction of the product properties: droplet size, density, viscosity, elasticity, yield stress, etc. These properties together with the concentrations of certain flavor chemicals form all physical and chemical properties which were correlated to the sensory attributes. There are in total 27 different sensory attributes, which were subdivided into taste, odor, appearance and mouth-feel categories. There are 13 input variables which contain processing variables and product formulation variables. The framework was used to answer the following question: can product creaminess be increased while the oil concentration is kept to a minimum? Full fat mayonnaises with oil fractions of 78 – 82 wt%, are evaluated to score on average two points higher on the sensory scale for creaminess than mayonnaises with 65 wt% oil. The outcome of this exercise was that several combinations of input variables for the manufacturing of a mayonnaise with 65 wt% oil were able to reach the same creaminess scores as for the 78 – 82 wt% mayonnaises.

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Synthesis of indirect work exchanger network based on transshipment model

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Energy is a major concern in the 21st century, the worldwide demand of which is predicted to rise by 57% during 2004-2030. The two common forms of energy in chemical plants are heat and work. As work is much more expensive than heat, work exchanger network (WEN) is an important part of energy recovery system, the design level of which will have significant influence on energy consumption in process system. M.S.Razib et al. [1] propose a superstructure for the WEN configuration and develop a MINLP to minimize the total annualized cost for a constant speed of the single shaft on 2-stream single-shaft-turbine-compressor (SSTC) units. Furthermore, Viviani C. Onishi et al. [2] introduce a multi-stage superstructure to optimize WEN configuration with heat integration simultaneously at a constant speed of the single shaft for SSTC.

The synthesis of indirect work exchanger network based on transshipment model is first studied in this paper considering the speed of single shaft as the variable. Compared with superstructure method, the transshipment model is more simple to obtain the minimum utility consumption taken as the objective function, which is also easier to get the optimized WEN configuration. The proposed approach for WEN synthesis is analogous to the traditional synthesis of heat exchanger network (HENs), which is an LP mathematical model applied to isothermal process and an NLP model in adiabatic process. Firstly, the minimum pressure difference ( ) is set based on experience and then all the streams are divided into several pressure intervals, also called sub-networks. Secondly, the energy balance is calculated in every sub-network according to the analysis of work cascade in both isothermal process and adiabatic process. Therefore, an initial work exchanger network is obtained. Thirdly, the relationship expression between the speed of axes and work recovery efficiency is established. The work recovery efficiency is changed by adjusting the speed of axes in order to decrease utility consumption and optimize the network structure. Finally, this method is proved to be feasible and effective by two examples.

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Development of sustainable CO2 conversion processes for the methanol production

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Utilization of CO2 feedstock through CO2conversion for producing valuable chemicals, as an alternative to sequestration of the captured CO2is attracting increasing attention from 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. Their net CO2 flows and methanol production costs were evaluated using ECON® and compared with those of the conventional methanol plant, which uses two-stage reforming. It was verified that the combined reforming process had 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.

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Optimal Design of Algae Biorefinery Processing Networks for the production of Protein, Ethanol and Biodiesel

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Sustainability in particular resource availability is a serious challenge to economic growth of chemical/biochemical industries. This motivates the development of technologies for utilizing more sustainable and renewable feedstock. This project is focusing on algae as an alternative renewable feedstock for manufacturing products including proteins, bioethanol and biodiesel products.

In development of algae biorefinery, there are a number of alternatives potentially available to choose from depending on types of algae and the processing technologies used to produce biodiesel, glycerol, ethanol and protein-based compounds. One of the challenges in identifying optimal algal biorefinery alternative is underlying uncertainties in data used for comparison and evaluation such as the volatility of market prices, process conversion and yields due to immature technologies, etc. Therefore, it is important to use a methodological approach at early stage design phase that can deal with uncertainties systematically and screen and identify the optimal designs. The design decision is complicated due to multi-criteria nature of objective function that includes techno-economic, environmental impact, and sustainability metrics.

In this study, a systematic framework that uses superstructure-based optimization is used to identify the optimal algal biorefinery concept under raw material composition and product uncertainties. First, a superstructure representing design space of algal biorefinery is developed. Next, the database (generic model and parameters and data) is collected to represent the algae biorefinery processing various types of algae feedstock to produce biodiesel, ethanol and protein-based compounds. The superstructure which is formed by the combination of the alternatives (types of feedstock, technologies, and products) together with the collected data, is then mathematically formulated as optimization problem and solved to identify the optimal designs with respect to techno-economic constraint under market prices uncertainty.

Using the framework, many processing network alternatives are generated and evaluated at their optimality resulting in the identification of the optimal processing paths. The generated database and superstructure provides a versatile process synthesis toolbox used in designing future and sustainable algae biorefinery.

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Design and Optimization of a Consolidated Bioprocessing Plant for the Production of Bioethanol

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The response to an uncertain energy future using petroleum based products has led to an increase in the study of renewable energy sources. Of these alternative energy sources, ethanol produced from biomass is a promising option. While many methods of biomass conversion exist, one interesting option involves the use of biochemical pathways which typically include enzyme hydrolysis and fermentation. However, the use of enzymes is expensive and account for a large percentage of the operating cost of the plant. To eliminate this cost, an alternative conversion pathway termed consolidated bioprocessing (CBP) can be considered.

Consolidated bioprocessing involves the conversion of cellulosic biomass to a desired product using an organism capable of simultaneous hydrolysis and fermentation, removing the need for enzyme addition.1 Many possible organisms are available for the conversion of cellulose, including Clostridium thermocellum and Escherichia coli.2,3 Some CBP organisms are capable of fermenting xylose as well, but recent studies have shown a higher conversion of xylose can be achieved if fermented separately with organisms such as recombinant Saccharomyces cerevisiae.4 A combination approach of CBP and xylose fermentation may lead to a more profitable bioethanol plant.

This study looks to design and optimize a bioethanol production process utilizing C. thermocellum and Thermoanaerobacterium saccharolyticum for the consolidated bioprocessing of cellulose and a separate pathway for the conversion of xylose using S. cerevisiae.5 The objective of the study is to minimize the ethanol selling price associated with the process, allowing for choices in biomass feed and corresponding pretreatment technologies. In addition, energy integration and water conservation strategies will be investigated to ensure a sustainable a process as possible. Finally, local and global sensitivity analysis will be performed to determine the key parameters affecting the economic viability of a CBP based bioethanol production plant.

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Model-based optimal design of a hydroformylation process with catalyst recovery by a thermomorphic solvent system

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Hydroformylation is one of the largest-volume homogeneously catalyzed reactions in the chemical industries. It converts olefins and synthesis gas to aldehydes, where the linear aldehyde is preferred. For a profitable process the selectivity with respect to the linear aldehyde and the recovery of the homogeneous rhodium catalyst are the most important goals. The selectivity depends mainly on the used ligand. For efficient catalyst recovery several new solvent systems have been proposed recently. In the present work we make use of a thermomorphic solvent system (TMS), which changes its miscibility behavior with changing temperature. Under reaction conditions the solvent system is a homogeneous mixture. By decreasing the temperature liquid-liquid phase splitting is induced in the TMS system [1]. In the polar phase the catalyst is dissolved and recycled to the reactor, while in the apolar phase the products and the non-converted educts are present and can be further separated via downstream processing.

For this process a dynamic optimization of the hydroformylation reactor embedded into the overall process was carried out. Thereby, optimal dosing strategies for the reactants distributed along the reactor have been derived. The underlying methodology considers the manipulation of the thermodynamic states of a matter element during its travel through the reactor by adjusting the external mass and energy fluxes [2]. After calculating the optimal control profiles the optimal fluxes are approximated as good as possible for achieving an optimal technical reactor. Thereby, various non-idealities of a real reactor have to be considered, including finite gas-liquid mass transfer rates and non-ideal residence time behavior.

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Synthetic Methane from CO2: Dynamic Optimization of the Sabatier Process for Power-to-Gas Applications

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Although discovered over a century ago, the main industrial use of the Sabatier reaction has been limited to purification steps in different chemical processes (e.g. H2 production, ammonia synthesis). Recently, CO2 methanation attracted increased attention as a promising key technology in the Power-to-Gas (P2G) process chain. It utilizes CO2 from biogas plants or coal fired power plants to convert H2 produced from renewable energy sources (Wind Energy, Surplus Electricity, Electrolysis) to synthetic methane, which can be easily fed into existing natural gas grids by which it can be stored and distributed.

There are several studies in literature that deal with the Sabatier reaction. They focus mainly on catalyst preparation, determination of the reaction kinetics or the investigation of the catalytic mechanism. But only little work has been done so far with regard to the optimal design of the Sabatier reactor for P2G applications. For this reason, here we investigate the optimal reactor design for CO2 methanation based on the flux-oriented "Elementary Process Functions (EPF) methodology. This approach was developed by our group and successfully applied in several reactor and process design studies including catalytic gas phase syntheses and gas-liquid reactions [1-3]. Based on our EPF methodology, we will demonstrate the optimization potentials of the Sabatier process aiming at minimizing the production costs of synthetic methane.

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[381]

Inter-process Heat Integration by Coordination among Agent Systems for Heat Exchanger Network Design

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Pinch technology is one of the commonly-used energy-saving technologies in chemical industries. We have proposed a simulation framework using multiagent into the design of heat exchanger network (HEN) to save the energy usage and to reduce the emissions of greenhouse gases. We set up several HEN Design Agents and each agents had different strategy to search candidate segments of HEN to modify. In our previous study, HENs for only a single process was optimized by the multiagent system at a time. However in general, there are some neighboring chemical processes in a site. The inter-process heat integration, in which heat giving and heat receiving between a process and the others, is effective for energy-saving in addition to the internal heat integration in a single process.

In this study, we introduced Coordinator agent within the multiagent framework to achieve both inner-process and inter-process heat integration simultaneously.

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Design and synthesis of batch processing plants: A consideration of utility aspect and using a robust scheduling platform

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The increasing interest in multipurposebatch plants is evident because of their inherent flexibility to cope with everchanging market environment. These plants are easily reconfigured for product modifications, to cover a wide range of operating conditions and suitability to produce different products within the same facility. Heating and cooling are unavoidable aspects of many chemical processing facilities, with operations where heat is generated and others where heat is required. It is because of this occurrence that heat integration becomes a possibility for reducing utility requirements. Not much is available in published literature on addressing design and synthesis of multipurpose batch plants considering heat integration. Moreover, the published work is based on discrete time representation for the scheduling model, thereby creating difficulty in solving large scale problems.The aim of this contribution is to address design, synthesis and scheduling simultaneously with the consideration of economic savings in utility requirements, while considering both the cost of the auxiliary structures and the design of the utility circuits and associated piping costs. The recent design and synthesis model by Seid and Majozi (2013) is extended to incorporate the design of the associated utility facility, since it is proven to result in better design objective and computational efficiencies. Additional feature of the proposed model is the determination of optimal pipe connection between processing equipments. The problem is formulated as a Mixed Integer NonLinear Program (MINLP) where binary variables are used for equipment, operational and topological choices, and continuous variables define the equipment capacities, heating, cooling and utility requirement in processes, as well as the amounts of material within the overall process. The nonlinearity in the model is due to the consideration of nonlinear cost function for equipment, heat exchanger and utility. The model is implemented in case study in order to demonstrate its application. From the case study, the profit is increased by 20% and the total utility requirement is reduced by 41.1% for the design and synthesis of energy integrated batch plant compared to the basic design.

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A Novel Approach for the Identification of Economic Opportunities within the Framework of a Biorefinery

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The design of multiple-feedstock multiple-product integrated biorefineries requires the evaluation of many different conversion pathways in order to (i) estimate production costs for a given product and (ii) identify the most attractive set of products and processing routes. Approaches such as detailed techno-economic analysis of specific feedstock-product production routes and development and mathematical optimization of biomass conversion superstructures have been successfully used to analyze biorefineries that have a priori fixed, and limited in size, set of target products. However, they are not practical when the set of potential products is very large or is not well defined, motivating the need for more flexible approaches for the early evaluation of processing ideas for the production of novel chemicals and materials from biomass. In this paper, we present a novel approach for the assessment of new processing ideas within the framework of a biorefinery. The approach is based on decomposing the production of biomass-based products in a demand and a supply problem that are linked through a set of intermediate compounds. The supply problem focuses on the fractionation of biomass into its elementary components (i.e. carbohydrates, lignin, proteins, etc.) through a sequence of pre-treatment technologies. A rational scheme for sequencing these technologies is proposed, and the intermediate and outlet streams resulting from this sequence of pre-treatments constitute the basis for the specified set of intermediate compounds. Alternative flowsheets for each of the steps of the pre-treatment sequence are built-in in a computer-aided collaborative environment, constructed in Aspen Plus. These pre-treatment sequences are then combined to create various biomass fractionation pathways that result in streams of intermediate compounds that differ in their degree of processing (e.g. polymeric or monomeric sugars), their quality (e.g. concentration of major components, presence of known inhibitors to downstream processes) and their cost. The demand side problem focuses on evaluating technologies that upgrade these set of streams of intermediate compounds into (novel) platform chemicals. On the basis that the cost of these platform chemicals is dominated by the total cost of the starting materials, the potential of a new processing idea or compound, is initially assessed by screening the available streams of intermediate compounds, using simple evaluations that consider their cost as estimated by the supply side problem and the yields that are achievable with a stream of that quality. If the processing idea is regarded as promising, then further evaluation with more processing details and complex metrics is conducted, and recommendations for experimental research are proposed. The proposed framework and the computer-aided collaborative environment are demonstrated through the evaluation of thermochemical and biological processes for the upgrade of the carbohydrates, obtained from the fractionation of date palm wastes.

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Integrated Design and Control of Semicontinuous Processes Using Mixed Integer Nonlinear Dynamic Optimization

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Process intensification techniques aim to reduce equipment sizes, improve process efficiencies and increase process profitability. Semicontinuous separation is one intensification strategy that is capable of reducing the capital costs of processes that require separation of three components by distillation. Semicontinuous separations are particularly beneficial for biofuel production networks in which many small-scale, distributed plants with low capital costs are desired. Semicontinuous separation utilizes a storage tank integrated with a single distillation column to achieve ternary purification, instead of the two distillation columns typically required in a conventional system. In the semicontinuous configuration, a side stream of the distillation column is recycled back to the tank (which initially holds the feed), while the contents of the tank are simultaneously fed to the column. Therefore, the composition and the flow rate of the feed to the column changes over the cycle time of the process. The system is control driven, working in three distinct modes of operation: charging, processing and discharging. To design a semicontinuous system for any arbitrary ternary mixture, appropriate design parameters such as number of stages, feed and side draw locations, storage tank volume and controller settings must be determined simultaneously and since the performance is highly sensitive to these parameters, optimization is crucial in order to obtain a profitable system. Classic dynamic optimization is a one option for this simultaneous design and control problem. However, since semicontinuous systems are highly complex (multi-modal limit cycles, high number of integer variables and expensive computational times) all previous attempts at dynamic optimization over the past decade have been limited to stochastic methods such as particle swarm optimization and/or limited to subsets of decision variables. In this work, a methodology for the synthesis of semicontinuous systems is presented using a deterministic mixed integer nonlinear dynamic optimization strategy for the first time. The separation of benzene, toluene and o-xylene is selected as a case study and the system is modeled in gPROMS v4. The outer approximation method with equality relaxation and augmented penalty method is used to solve the MINLP problem. An economic analysis is performed to compare the conventional distillation systems and the optimally designed semicontinuous systems.

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A Computational Platform for Simulation, Design and Analysis of a Poly(Lactic) Acid Production Process From Different Lignocellulosic Raw Materials

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Polylactic acid (PLA), a biodegradable poly hydroxy alkanoate (PHA), is a promising replacement for synthetic polymer. The advantages of polylactic acid are its high tensile strength, high modulus, thermoplastic property, biodegradability and bioenvironmental compatibility/absorbability. There are several technical challenges involved in the production of high-molecular weight PLA polymers. First, it is necessary to remove water from the product since the esterification reactions are highly reversible. This is especially challenging because the polymer is hydrophilic. One industrial solution to this problem is to produce the polymer using lactide intermediate instead of raw lactic acid. A second technical challenge is to maintain the proper steric structures in the final product. Lactic acid is composed of two enantiomers; D-lactic acid and L-lactic acid. Biological activity strongly favors the L-lactic acid units. For biodegradability, it the amount of D-lactic acid units in the polymer (average block length of these units) should be minimized. The present work presents a computational platform for the simulation, design and analysis of the polyLactic (PLA) acid production process using different lignocellulosic raw materials. The computational platform considers three main reactive-separation processes: 1) the bio-conversion process, where an hydrolysis-saccharification-culture process to produce the inoculated hydrolysate is coupled with a fermentation-separation process producing the broth with crude lactic acid; 2) the purification process, where a sequence of conventional and reactive distillation columns to perform the esterification and hydrolysis reactions, respectively, are used to produce a polymer grade lactic acid; and 3) the polymerization process, where a ring-opening polymerization reaction scheme to produce high molecular weight PLA is carried out. The implementation of the platform in a systematic manner allowed the evaluation of various readily available mono and disaccharide materials to produce PLA i.e., glucose (dextrose) and glucose syrup as end product of starch conversion; maltose as a product from barley malt or other source; sucrose as end product of beet and cane sugar production and lactose as a constituent of whey. The global PLA production processes showed different operating scenarios depending strongly of the content of glucose and xylose into the lignocellulosic raw material. The results show that with a higher concentration of glucose the molecular weight of the PLA produced increased. However, the operation of the purification section, that is, the reactive distillation section should be carried out carefully in order to obtain a purified lactic acid near to 88% mass fraction. The highest molecular weight for PLA in the a global process configuration was found considering a continuous fermentation and a raw material pretreated to have equal concentration of glucose and xylose.

[407]

Simultaneous Design of Desalination Plants and Distribution Water Network

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Northern Chile is characterized by significant mineral resources, particularly copper, nitrate, lithium, molybdenum, rhenium, among others. Moreover, these resources are located in the Atacama Desert, the driest in the world. Water resources are exhausted, but Chile has an extensive coast from where to get water. Then, any new operation or expansion of a current operation must use seawater. The distance from the coast to mining operations ranging from a few kilometers to about 300 kilometers, but even more significant, these operations can be found from 600 to 4,000 meters above sea level. Then, the cost of transporting desalinated water can be four times the cost of desalination.

This paper presents a methodology to design the system of desalination plant and desalinated water transport. The objective is to determine the location and size of desalination plants and the water distribution system that minimizes capital and operational costs. The methodology uses a superstructure that represents the set of alternatives on which to find the optimal solution. A mathematical model is generated to represent the desalination plant and water distribution system. The end model corresponds to a MINLP problem which is solved with commercial software for the global solution. A case study is used to demonstrate the applicability of the methodology developed.

[408]

Optimal Design of Microfluidic Platforms for Diffusion-Based PCR for "One-Pot" Analysis of Cells

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Genetic analysis starting with cell samples often requires multi-step processing including cell lysis, DNA isolation/purification, and polymerase chain reaction (PCR) based assays. In recent times such analysis are conducted on a microfluidic platform; however, the compatibility among various steps often demands complicated procedure and complex device structure. We have developed a microfluidic device that permits "one-pot" strategy for multi-step PCR analysis starting from cells (i.e. using one reactor for successive reactions without separation and purification) [1]. The strategy exploits diffusivity differences, effectively replacing the smaller molecules in the reaction chamber by diffusion while retaining DNA molecules inside. This simple scheme effectively removes reagents from the previous step to avoid interference and thus permits multi-step processing in the same reaction chamber. Our approach shows high efficiency for PCR and potential for a wide range of genetic analysis including assays based on single cells. So far we have demonstrated a simple scheme for conducting microfluidic PCR starting from cells, taking advantage of the difference in the diffusivity between genomic DNA and various reagent/intracellular molecules. Our microfluidic device has a relatively simple structure that includes a reaction chamber connected with two loading chambers on both sides. Closing two-layer valves could cut off the connections between the reaction chamber and the two loading chambers. The lysis buffer and the PCR mix are introduced into the chamber by concentration-gradient-driven diffusion. During such diffusion, the new solution replaces the solution and molecules from the previous step without removing the slow-diffusing genomic DNA. The single chamber ("one-pot") design drastically minimizes the complexity of the microfluidic device. We envision that this may be a general approach for on-chip multi-step assays on genomic DNAs. In our paper [1] we argued that the three commonly known strategies to alleviate the impact of cell pretreatment on PCR had serious shortcomings. The three strategies are: (a) Use an isolation step to remove lysis reagent and undesired intracellular molecules while preserving nucleic acids. The associated isolation step increased the complexity of the procedure and chip design. (b) Use lysis methods, such as freeze-thaw or heating, that interfere with PCR to a less degree than surfactants. However, these methods are less efficient than surfactant-based lysis. (c) Use Direct PCR kit based on Phusion polymerase that is tolerant to surfactant based lysis reagents, but this commonly used fluorescence-based quantification is impossible with the Phusion polymerase system. There is little doubt that microfluidic strategies that permit simple operation and device design and are compatible with Taq polymerase are highly in demand. In this presentation, we discuss some optimization-based (Process Systems Engineering) microfluidic platform designs, which are more efficient than the current one we have developed. We will discuss reaction-diffusion modeling (parabolic partial differential equations in 2-D and 3-D) while optimizing the process conditions. In the future we will build these devices to efficiently carry out PCR; the data collected would also be employed to validate our modeling effort.

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[411]

A Systematic Methodology for Optimal Mixture Design in an Integrated Biorefinery

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In the past decades, utilization of biomass as an alternative renewable energy source is seen as a potential sustainable solution for solving global environmental issues and reducing dependency on fossil fuels. Through various conversion pathways, biomass can be utilised to produce power, heat and higher value products such as biochemicals and biomaterials. To date, a large amount of potential biomass conversion pathways and technologies are available commercially to convert biomass into a wide range of potential products. However, minimal effort has been done on addressing the design of end products of the integrated biorefinery. In order to address this issue, there is a need to identify the desired products which can be produced by the optimal conversion pathway. In addition, there are situations when the desired product comes as a mixture/blend of chemicals rather than a single molecule. Generally, these mixtures contain one or more liquid chemicals as the main ingredient and a set of additional chemicals which acts as additives. The main ingredient performs the key functionalities of the mixture while the additives enhance the quality of the mixture. Hence, a systematic methodology is required to design a mixture/blended product efficiently. In this work, a two-stage optimization approach is developed to identify the optimal conversion pathways in an integrated biorefinery that convert biomass into optimal mixture. In the first stage, mixture design is done by computer aided molecular/mixture design (CAMD) technique. CAMD technique is a reverse engineering approach which predicts the molecules using property prediction models. In order to design an optimal mixture by using CAMD technique, the desired mixture attributes are first expressed in terms of physical properties. In the next step, the main ingredient of the mixture is identified from the target properties. This is followed by determining the additive to form the mixture with the main ingredient. Hence, the optimal mixture that possesses optimal product properties can be designed by mixing the identified main ingredients and additives together. In the second stage, the optimal conversion pathway is determined via superstructural mathematical optimization approach. Note that the optimum conversion pathway based on different optimization objective (e.g. highest product yield, lowest environmental impact etc.) can be determined by utilizing the optimisation approach. By utilising the developed methodlogy, an optimal blended biofuel in terms of optimal target properties is designed. The optimal blended biofuel with highest research octane number (RON) is designed as a mixture of molecules which consists of a main ingredient and an additive. At the same time, the optimal conversion pathway in terms of highest product yield which converts the palm-based biomass to the optimal blended biofuel is also identified.

[414]

A systematic visual approach to ionic liquid design for carbon dioxide capture

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Carbon capture and storage (CCS) is a vital technology to mitigate industrial CO2 emissions, which is mainly generated in power plants. Currently, post-combustion capture based on aqueous amine scrubbing is considered as the most suitable technology for CO2 capture. However, the use of amine for CO2 capture has some disadvantages, such as high energy requirement for solvent regeneration, high vapour pressure which causes subsequent solvent loss, degradation of solvent. Recently, ionic liquids (ILs) are considered as a possible alternative to amine solvents, because they have negligible vapour pressure, high thermal stability, and flexibility to tune the properties by matching cations and anions. ILs refer to organic salts that are liquids close to ambient conditions, which consist of relatively large organic cations and inorganic or organic anions of smaller size and asymmetrical shape. It is estimated that there are as many as 106 possible unique cation and anion combinations. Therefore, time and expense required to determine the optimal ILs specifically for CO2 absorption is unaffordable. The main focus of this work is to develop a systematic property based visual approach to synthesise and design ILs, specifically for carbon capture purpose. The visual tool is able to design ionic liquids and provide a list of potential candidates that satisfy all constraints considered. This can be a screening tool prior to the experimental work, and hence reduce time and cost required for experiments. In this approach, the design problem is visualised on a ternary diagram through property clustering techniques, which is generally based on the use of property operators. The relationships between properties are mapped into low-dimensional domain to form property clusters, and hence allow the visualisation of the problem. On the ternary diagram, all potential ILs will be identified, along with their respective properties. The approach utilises property prediction models (e.g. group contribution method) to estimate the thermophysical properties of ILs. However, most of the property prediction models for ILs available currently do not cover wide range of ILs, which may cause deviations in predicting properties. In order to improve the property prediction, the proposed approach is able to identify and take the experimental data into prediction model. The property prediction models employed in this approach is modified, such that new experimental data is first identified, and then used to improve the existing models. This can provide data for new IL building blocks (i.e. cations and anions). An illustrative case study is solved to demonstrate the developed approach.

[420]

Intensification of C5 separation process by heat integration and thermal coupling

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C5 fraction, which accounts for 15-25% in naphtha, consists of molecules such as isoprene (IP), pentadiene (PD), cyclopentene(CP), and cyclopentadiene (CPD) can be used to manufacture petroleum resin and other high value-added products. Yet it is often burned as fuel and not fully utilized because separation of these products with close boiling points is difficult. One common process is to react CPD itself to form di-cyclopentadiene (DCPD) so that it can be separated from the other C5 molecules. Extractive distillation was also used to recover alkynes from light ends. Such a process involves use of multiple separation columns and reactors. Furthermore, it was found that the reactor is highly coupled with one of the separation columns by a recycle stream, leading to snowball effect and difficulty in control. Hence a wide range of opportunities for process intensification and integration was available. It was found that the entire separation process can be substantially simplified by reducing number of reaction zones from 2 to 1 and number of columns from 8 to 6. Such a simplification increases product concentration of DCPD from a range between 85wt% and 92wt% to 99wt%, while maintains the high purity (>99.75wt%) for the IP stream and specified purity (>89.90wt%) for the PD plus CP stream. This process can be further simplified by using thermal coupling and external heat integration. Such simplifications and intensified techniques lead to substantial reduction in capital costs, energy costs as well as process operability.

[462]

Conceptual Design of Post-Combustion CO2 Capture Processes - Packed Columns and Membrane Technologies

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Since CO2 is concerned to be one relevant greenhouse gas, the CO2-emissions have to be reduced significantly. Currently, state of the art for CO2 removal is the chemical absorption using aqueous amine solutions (e.g. monoethanolamine). The overall CO2 capture process consists of two major parts: absorption and regeneration. Due to the loss of process efficiency, caused by the high energy demand for the absorbent regeneration, large scale industrial application of CO2 capture is restricted. Therefore, techniques to design energy efficient process structures are needed.

One of those techniques is called hybrid processing. Hybrid processing generates intensified process configurations by combining at least two technologies for one separation task. Different operating windows and the differing operational flexibility of the technologies can offer an advantage for the process. Determination of such configurations is difficult due to the complexity of options involved. While methods and models for process design of such systems for vapor-liquid does exist, the application of these to gas-liquid still remains challenging. Furthermore, these methods are up to now mainly applied for conventional processing, like e.g. packed columns. This work expands these methods to intensified processing technologies.

In addition to the hybrid processing a second technique is applied. Here, process intensification is reached by use of intensified contacting devices, like membrane contactors, providing high mass transfer areas and outstanding operational flexibility. This intensification is different to the hybrid processing as it takes place on phase level and not on process level. An additional intensification on phase level can be achieved by applying a bio catalyst, like the enzyme carbonic anhydrase, which could lead to an increase in the reaction rate for absorption or desorption. It becomes apparent that by applying two different techniques simultaneously an integrated process intensification is conducted, showing the unique, complex and challenging nature of this work.

The approach to master this challenge is to reduce stepwise the number of involved options and to increase gradually the complexity in modeling. As a first step the search space has to be determined. Therefore, different solvents for the absorption as well as different membranes for the gas absorption and different devices for contacting the phases are evaluated. For this purpose, the comparison is based on short-cut models. These results are used to scale down the number of options ending up with promising process configurations. In a subsequent step the complexity is increased by use of detailed models for the most promising configurations. As there are no models available for the intensified technologies as well as for the contacting devices, new models have to be developed and validated against experimental data.

A process analysis of different configurations and intensification levels is performed and compared to a base-case process as a benchmark. This shows the potential of process intensification by hybrid processing or intensification on the phase level or a combination of both to fill the gap in industrial acceptance of the absorption based CO2 capture process.

[508]

Natural Gas to Liquid Transportation Fuels and Olefins (GTL+C2_C4)

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The United States faces major challenges towards the production of liquid transportation fuels and high value petrochemicals. High crude oil prices coupled with the volatility of the global oil market account for the economical challenges as the United States petroleum sector heavily depends on imports. Moreover, excessive greenhouse gas (GHG) emissions is an environmental concern since petroleum industries are responsible for 33% of the total CO2 emissions in the United States. These challenges can be addressed using domestically available feedstocks such as coal, biomass, natural gas, and municipal solid waste. Recent works have already shown that the production of liquid transportation fuels from different combinations of coal, biomass, natural gas, and municipal solid waste are economically viable alternatives to typical petroleum processes. However, high value petrochemicals, such as C2 to C4 olefins are important products of the refineries and are in high demand in the petrochemical commodities market. Therefore, alternative single or hybrid feedstock energy systems should also consider coproduction of C2 to C4 olefins with liquid transportation fuels. The primary C2 to C4 olefins, ethylene, propylene, and butadiene, are used as valuable intermediates in the petrochemical industry. Furthermore, cheap and abundant natural gas feedstock is available in the United States due to the advances in the shale gas industry. Therefore, this work considers the co-production of C2 to C4 olefins with liquid transportation fuels starting from a natural gas feedstock. An optimization based framework is used to perform a techno-economic and environmental assessment of a refinery that can convert natural gas to liquid transportation fuels and C2 to C4 olefins. Multiple natural gas conversion pathways are introduced in the process synthesis superstructure. The natural gas can be converted into synthesis gas (syngas) or other intermediates such as methanol or olefins. Syngas can be directed to either the Fischer-Tropsch hydrocarbon production section or methanol synthesis section. The raw Fischer-Tropsch hydrocarbons can be upgraded to fuel quality products using standard fractionation units or a ZSM-5 based catalytic reactor. Similarly, methanol can be converted to gasoline or olefins. The olefins can be purified to be sold as products or sent to an oligomerization process to be converted into gasoline and distillate. The CO2 produced in the plant can be vented, sequestered, or recycled back in the refinery. The optimum plant topology is determined by the optimization-based framework that consists of process synthesis and global optimization strategies. Simultaneous heat, power, and water integration is performed to keep utilities costs at minimum levels. The most preferable process (lowest cost or highest profit) is selected within this framework that produces liquid transportation fuels and C2 to C4 olefins. The tradeoffs between each alternative in the proposed superstructure are investigated. The effects of plant capacity, liquid fuels composition, and olefins production levels are investigated through different case studies. The key foundations, topological decisions, economical and environmental aspects observed within the case studies are outlined.

[534]

Optimization of ionic liquid recycling in Ionic Liquid-based Three Phase Partitioning processes

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The major bottleneck of the economic and technical viability of protein production processes is downstream processing, since the conventional methods to purify these biomolecules are time and cost consuming (Pei et al., 2009). In this way, Ionic Liquid-based Three Phase Partitioning (ILTPP) has been proposed as a novel technique to recover proteins at the liquid-liquid interface formed by ternary systems ionic liquid/salt/water, which combines the use of Ionic Liquid-based Aqueous Two Phase Systems (ILATPS) with results that are characteristic of Three Phase Partitioning (TPP) (Alvarez-Guerra and Irabien, 2014). However, the development of ILTPP processes highly depends on the consumption of the reagents involved, and especially of ionic liquid, because of its relative high price.

For this reason, the net consumption of ionic liquid in this process has been assessed in previous works, concluding that between 0.8 and 5% of the ionic liquid cannot be reused, depending on experimental conditions. Therefore, two additional steps to enhance the ionic liquid recyclability have been considered: the increase of the salt concentration to reduce the ionic liquid fraction in the waste stream, and the water removal by means of evaporation to increase the fraction of liquid phases that can be recirculated in the process (Alvarez-Guerra et al., 2014). Nevertheless, the previous studies have assessed these additional recovery steps individually.

The aim of this work is the economic optimization of the ionic liquid recovery in ILTPP processes so that the costs associated with this recycling, which constitute the objective function, are minimized. This approach makes it possible to analyze simultaneously all the different alternatives to recycle the ionic liquid in the most efficient way: the individual additional recovery steps previously mentioned, a combination of them or the performance of the process without any of these steps. The main operational costs of the ILTPP process (independently whether the salt concentration is increased or not) considered in this work are the net consumptions of both the ionic liquid and salt, and when the alternative based on evaporation is considered, the energy required to remove the desired amount of water. Consequently, the process configuration and the experimental conditions that lead to the ionic liquid losses that minimize the operational costs of the process are identified.

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[540]

Life-Cycle Assessment Principles for the Integrated Product and Process Design of Polymers from CO2

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Today, polymers are usually synthesized from fossil-based feedstocks. As alternative and renewable carbon feedstock, carbon dioxide (CO2) has recently successfully been utilized as building block for polyols [1]. CO2 utilization for polymers has the potential to significantly reduce fossil resource depletion and CO2 emissions [2]. In addition to the direct utilization of CO2 as feedstock for polyols, CO2 can also be used indirectly to produce other chemicals in the polymer supply chain. Both direct and indirect utilization of CO2 provide novel degrees of freedom to achieve desired polymer properties.

The goal of this work is the simultaneous optimization of the polyol production supply chain and polyol properties with minimal environmental impacts. Environmental impacts are obtained by life cycle assessment (LCA). In this work, the carbon footprint is chosen as single LCA metric to avoid further complexity with multiple environmental objectives. The considered polyol properties (molar mass, glass transition temperature and hydroxyl value/OH number) are predicted from the polyol structure using quantitative structure property relationships (QSPR). Due to non-linear QSPR, the optimization problem is formulated as non-linear programming (NLP). Three feedstocks for polyols are considered: CO2, a CO2-based precursor and fossil-based propylene oxide. For each feedstock, alternative production processes are considered and a supply-chain superstructure is generated.

In the optimization of the supply chain, we have to consider that chemical processes usually provide more than one product. As example, feedstock CO2 might be captured from ammonia synthesis which thus produces the two products ammonia and CO2. To obtain a product-specific carbon footprint for polyols, greenhouse gas emissions of multi-product processes have to be allocated to the individual products. The various allocation approaches have received much attention in the LCA literature and were shown to lead to strongly varying product footprints [3]. We apply alternative allocation approaches to the optimization problem and derive general principles from allocation in LCA for environmental process-product design.

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[561]

Optimization-based methodology for wastewater treatment plant synthesis – a full scale retrofitting case study

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Wastewater treatment process synthesis can be defined as the step in the design of a wastewater treatment plant (WWTP) where the design engineer selects unit processes from a number of alternatives and interconnects them to create the process flow diagram. Process synthesis is also performed during retrofitting studies in the sense that a new task can be added to the existing treatment line or one or several existing processes can be changed as a result of the emerging needs. Existing WWTPs need retrofitting due to a number of reasons such as: change in the wastewater flow and composition, change in the effluent limitations, as well as changes in the wastewater treatment trends. For instance, increased nitrogen limitations in the regulations for the WWTP effluents gave rise to development of innovative nitrogen removal technologies including several nitritation-anammox processes mostly used for water streams resulting from sludge treatment. Similarly, recovery possibilities for clean water, energy and materials shifted the perception about wastewater towards being a valuable resource rather than being a waste. While the regulations change to impose stricter effluent limit values for the contaminants, the increasing population and the size of the cities put a barrier on the expansion of the existing wastewater treatment plants. Therefore, the retrofitting task has become a complex integrated decision making problem where a number of aspects are being contemplated in the early stage decision making. In this study we propose a superstructure optimization concept based on mathematical programming to manage the multi-criteria WWTP design/retrofit problem and generate novel and optimal network designs for domestic WWTPs. Alternative treatment technologies are represented in a superstructure; each of which is described by a generic model in terms of input-output mass balance. The superstructure is coupled with a database containing data for both performance and economics of the alternative technologies. The superstructure optimization problem is formulated as a Mixed Integer (Non)Linear Programming problem and solved in GAMS for different scenarios represented by different objective functions and constraint definitions. Finally, a full-scale wastewater treatment plant with approximately 70,000 m3 d-1 capacity, namely Avedøre WWTP located west of Copenhagen, in Denmark, is used as a case study in order to highlight the use of the framework.

[562]

An Integrated Framework for Controllability Assessment and Solvent Selection in Post-Combustion CO2 Capture Processes

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Lately, the consideration of different solvents in the optimization of absorption/desorption processes in CO2 capture research, such as process structure and size, topology of recycle streams within the flowsheet and solvent feed flowrates, to name a few, is receiving significant attention to further improve the process economics. However, such processes are essentially dynamic environments susceptible to variations in operating parameters (e.g., temperature, pressure, and composition drifts, solvent degradation and losses) and influence from exogenous disturbances (e.g., input flue gas composition). As such, absorption/desorption systems designed for optimal but constant operating conditions will divert from their designed operation if any of such parameters vary in time, a case often observed in industrial practice. The effects of different CO2 capture solvents in process design under operating variability that explicitly considers the controllability properties and the operability performance of the overall process system have yet to be addressed systematically.

The current work addresses the economic performance simultaneously with the static and dynamic controllability properties of amine based CO2 capture processes. Amine solvent candidates are introduced into a unified framework supporting optimal design while considering variations in process parameters and disturbances in process operation. The proposed framework consists of a process design and a nonlinear sensitivity analysis stage that evaluate process design and control structure configurations under the influence of multiple simultaneous parameter variations and/or exogenous disturbances. The absorption/desorption design stage involves a process synthesis approach employing reactive and non-reactive separation column modules of sufficient modeling detail and flexibility acquired through the implementation of an orthogonal collocation on finite elements (OCFE) approximation technique. The nonlinear sensitivity analysis stage investigates the steady-state and dynamic effects that process parameters and disturbances impose on the system for a given input-output control structure. The control scheme categorizes control objectives and preferences in the utilization of manipulated variables in a multivariable centralized fashion. Within this framework, alternative solvents of different chemical structure and physical properties are introduced in order to study their effects in optimal design and operability performance under operating conditions variations. The performed sensitivity analysis not only generates useful insights regarding the control structure selection and the range of parameter variations within which the solvents demonstrate optimum performance, but it also allows the adaptive modification of the process design characteristics in order to enhance process operability.

The proposed developments are illustrated in case studies considering amine solvents such as monoethanolamine (MEA), 2-amino-2-methyl-1-propanol (AMP) and diethanolamine (DEA) which are commonly used for CO2 capture. The thermodynamic behavior of the CO2-water-amine mixtures is described through pressure-loading relationships extracted from the Statistical Associating Fluid Theory for potentials of variable range (SAFT-VR). Various absorption/desorption structures are evaluated including recycle split streams, multi-pressure cascades etc., in view of the considered solvents.

[566]

Using Product Driven Process Synthesis in the Bio-refinery

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In the last fifteen years the bio-refining industry gained momentum and started offering an alternative to the petroleum based energy and chemicals industry. However to assure a profitable bio-refinery, a holistic view of all possible product classes (e.g. biomaterials, fuels, chemicals) into the bio-refining operation is imperative. It is clear that the design of a bio-refinery stands or falls by the grace of the design of the products it should produce.

In this work, we propose the use of the product-driven process synthesis (PDPS) methodology as a tool for structured decision making during the product and process design stage. The important decisions concern the specification of feed stream(s); the specification of product(s), and the specification of the operations required to transform the raw materials into products in such way that the overall design is economically attractive and that safety and environmental constraints are satisfied (Bongers and Almeida, 2012).

PDPS is a hierarchical product development methodology, originally developed to describe the process of making one (structured) product from several raw materials. However, when PDPS is applied in the field of bio-refinery, where multiple products are extracted from one starting raw material, a number of modifications to the method are required. This paper describes these PDPS modifications by using the sugar beet leaves, as a case study.

Sugar beet leaves form an excellent example for our bio-refinery. Often the sugar beet leaves are considered to be harvest waste, but the leaves contain a plethora of potentially interesting products. In the first level of the PDPS the so called Input-Output level is defined. The sugar beet leaves are decomposed into their compounds. Subsequently, a list of different compounds, often used in food applications, and their respective functionalities is designed. This list is expanded to include the prices of these compounds and the different technologies that can be used for their separation. With this information, the main compounds of interest are identified and the next steps of the PDPS can be taken, i.e. the formulation of task networks, the description of the operating windows and ultimately the conceptual process design.

Applying the modified-PDPS has several advantages. The pre-identification of the main compounds of interest allows for a risk assessment before going to research, and thus a risk reduction. In addition, it offers a well-defined platform for the design of an integrated bio- refinery, by combining different technologies that can be used for a selection of compounds.

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[569]

Integrating expanders into sub-ambient heat exchanger networks

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The concept of Appropriate Placement is fundamental in Pinch Analysis and addresses how different pieces of equipment can be integrated with heat recovery processes to ensure it results in energy savings, also referred to as Correct Integration.

The placement of expanders refers to the inlet temperature of expansion processes. Recently the appropriate placement of expanders has been discussed in literature [1-2] and formulated as the following heuristic rule: expansion provides cooling to the system and should thus preferably start at pinch temperature. However, such observations are not based on strict mathematical or thermodynamic analysis. When designing a heat exchanger network (HEN) including expanders, the application of the rule may not be straightforward.

Since both heat and power are involved, the objective of this work has been to minimize exergy consumption for the integrated processes. Actually, the study has resulted in a procedure for targeting minimum exergy consumption. The insight obtained from various case studies has been generalized and formulated as a set of theorems with corresponding assumptions. While establishing these targets, the optimal use of Pinch Expansion (expander inlet is at pinch temperature) will be identified and the corresponding possible split of streams into sub-streams (or branches) make the design task easy and straightforward.

Several challenges exist when applying the rule about "Pinch Expansion" for integrating expanders into a HEN: (1) the streams to be expanded are included in the HEN, thus the heat demand for streams is changing; (2) the role of a stream (as a hot or cold stream) to be expanded may change after expansion; (3) Pinch Expansion may produce more cooling than required, thus stream splitting is required; and (4) the heating or cooling of a stream with pressure manipulation may create new pinch points. The integration of expanders into HENs is thus a rather complex problem.

The objective of this paper is to develop design guidelines for integrating expanders into HENs with a target of minimizing exergy consumption. Theorems are presented to indicate when Pinch Expansion is preferred with respect to exergy consumption. Graphical methods are used to illustrate how Pinch Expansion can be implemented. A design procedure that achieves the minimum exergy target is presented. The procedure has been applied to a membrane process for separation of CO2 from flue gas. The specific energy consumption for CO2 separation is reduced by 14%.

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[581]

Water free XTL processes: is it possible and at what cost?

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Coal to Liquid (CTL) processes have received renewed attention in recent years. However, these processes face significance challenges in terms of the very high water consumption, and high CO2 emissions if Carbon Capture and Sequestration is not applied. Although the water consumption of a CTL process can be reduced when a closed cooling water system is applied and air cooling is used instead of cooling water, the overall mass balance for a CTL process still requires water as a feedstock(, to provide the hydrogen needed in the process. Our previous analysis shows that 1.3 tons of water is needed as feedstock to produce one ton of CH2 assuming coal as pure carbon. On the other hand, when biomass is used in the XTL (X= Coal, Biomass, Natural Gas, Waste etc.) process, there is a potential that water is actually produced from the process. As the composition of biomass is close to a very low quality coal, it raises questions that for some low quality coal, it is possible that extra water is not really needed for the overall mass balance.

In this contribution, basic process synthesis tools including mass and energy balances are applied to investigate the possibility of a water free XTL process. It is found that as long as there is hydrogen in the feedstock, a water free XTL process is possible at the cost of a lower carbon efficiency as the result of imbalance of the hydrogen / carbon ratio in the feed. The region where a water free XTL process can be achieved with reasonable carbon efficiency is investigated. Addition of water in the feed can improve the carbon efficiency of the process, therefore a balance between the water requirements and carbon dioxide produced needs to be considered.

[586]

Energy and Yield Evaluation of an Alcohols and Hydrocarbons Production Plant using Rh-based Catalysts with Different Promoters

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Synthesis gas (syngas) is mainly constituted by carbon monoxide (CO) and hydrogen gas (H2) and is produced mostly through biomass gasification and methane (CH4) reforming. The chemical route to directly produce ethanol and higher alcohols, is gaining space in the last decade as a possible route to produce synthetic fuels and additives [1,2]. This kind of process presents a series of advantages as: the short-time reaction, abundant and lower price feedstocks, the use of lignin (a biomass component that is hardly used) and the almost complete conversion of syngas, having the potential to exceed ethanol production by fermentative route [3].

Among several catalysts, Rh is known by occupying an interesting position in periodic table, between those metal that dissociate carbon monoxide forming long-chain hydrocarbons (Fe, Co) and those who does not dissociate CO and produce methanol (Pd, Pt, Ir), so the Rh-based catalysts can form long-chain oxygenate compounds from CO hydrogenation [4]. However, one of the drawbacks of Rh-based catalysts is the high selectivity to hydrocarbons, generally varying in its chain size from C1-C5.

In this work four different cases were evaluated changing the Rh-based catalyst (RhFe, RhLa, RhLa and RhLaFeV [5]). Aiming to produce ethanol, a singular process layout (a small-scale plant with capacity to process 100 kmol/h of syngas) was developed using the commercial Simulator Aspen Plus v7.3. In such design we tried to take advantage of Rh characteristics as catalyst, producing, besides Ethanol (> 99% wt.) and Methanol (> 90% wt.) Liquified Petroleum GAS (LPG, a mixture of C2H6, C3H8 and C4H10, > 99% wt.) that can be used as fuel (for selling or as energy in the process) and Pentane (> 99% wt.) a solvent commonly used in industry.

The process design took into account reactor selectivity and conversion, the four catalysts were compared and highlighted regarding energy usage and products yield, in addition, the downstream process were optimized, searching, through sensitivity analysis, the best configuration of separation steps.

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Production of enriched air by water degassing for process intensification: experimental results and relative modeling

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A new kind of chemical processes intensification can be obtained by the production of enriched air (EA) from degassing of air saturated water by pressure or temperature action [1]. This possibility is economically feasible in some chemical plants or process where great quantity of hot water are required, for example as in multi-effect distillation (MED) technology in the seawater desalination plant.

This intensification is based on the production of a flow of enriched air, i.e. an oxygen/nitrogen mixture with an amount of O2 in the range of 22-35 vol.%. Enriched air can therefore be used to reduce the variable costs of the intensified plants as well as to reduce the volume of process facilities dedicated to steam generation or to directly increase the net operating margin as additional product (industrial or medical gas). The basic principle is based on the different Henry's constant of oxygen and nitrogen in water, which can reach the value 65 vol.% of nitrogen and 35 vol.% of oxygen [2]. When the temperature increase and/or pressure decrease, the content of N2, O2 decreases due to their consequent release into the atmosphere.

Proper experimental tests were carried out in a laboratory batch plant in order to optimize the two main operative parameters of this operation, i.e. T and P. This plant is composed by: (I) a vessel filled with water taken from the municipal water in order to equilibrate with N2 and O2 present in the atmosphere; (II) a batch reactor filled with 6 L of water taken from the vessel and able to work at 55<T<75°C and 260<P<500 torr; (III) a m-GC for the measure of the composition of the EA produced.

Experimental results highlight that the degassing process is not a flash operation, in fact also if the mixture water/N2/O2 is in not equilibrium conditions (for example water from room temperature is heated till 80°C), EA is not obtained simultaneously with the increasing of temperature. For this reason, the production of EA in function of the time in different T and P conditions was studied. The results in terms of %O2 reached in function of time at T = 65 °C and different pressure will be presented.

These data shows that the rate of %O2 obtained increases in decreasing pressure applied in the reactor at constant temperature; the same data have been elaborated for the modeling of this technology by suitable simulation software (PROII and Dynsim) in order to validate and simulate the EA production process obtaining the optimal conditions for the application in different chemical processes.

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[593]

Computer-aided process analysis of integrated biodiesel processes incorporating reactive distillation and organic solvent nanofiltration

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Biodiesel based on renewable resources shows a great potential as alternative fuel in future. Until now no economic production of biodiesel is possible because of high raw material costs of virgin vegetable oil. A promising and cheap alternative as feedstock are waste cooking oils. The drawback of these low-quality oils is the high amount of free fatty acids (FFA) which tend to hydrolyse under the alkaline conditions in the transesterification reaction of biodiesel. Therefore, the amount of FFA in the waste cooking oil has to be minimised in a pre-treatment step before it is fed to the transesterification reactor. One possibility is the esterification of FFA with an alcohol. Since this reaction is equilibrium limited the application of reactive distillation (RD) is favourable. However, the concentration of FFA in the column is low due to a high amount of non-reacting triglycerides in the waste cooking oil which might lead to mass transfer limitations and therefore, a restricted operation window for the RD. Furthermore, the composition of waste cooking oil is fluctuating. To overcome this challenges and widen the operation window of RD an integrated process combining RD with organic solvent nanofiltration (OSN) is proposed. OSN allows an energy efficient separation of FFA and triglycerides and could be used to adapt the waste cooking oil.

To enable this integrated process a detailed investigation is performed. In a first step both unit-operations were investigated experimentally to provide necessary data. Since separation performance in OSN depends on various factors, like molecular size of components, solubility parameters etc. no prediction of separation efficiency is possible and missing parameters has to be determined experimentally. Therefore, a membrane screening was performed and the influence of different solvents on the performance was investigated. Furthermore, RD experiments were performed to determine the operation parameters for the column process. In the second step a rigorous model for the integrated process consisting of a RD column and a OSN superstructure was developed in Aspen Custom Modeller (ACM) for the purpose of process analysis and process design. The OSN superstructure comprises of various membrane modules which could be connected in parallel or series and could be operated at different temperature and pressure. Model validation was done by the experimental results. Within process analysis, the influence of different operating points of RD or OSN on the process performance is determined and feasible operating windows for different integrated process configurations are identified. Based on this a detailed process design is performed considering performance indicators such as yield and purity as well as energy efficiency to determine the most promising process configuration. Finally the best configuration of the integrated process is compared to a base case design.

[605]

Optimization of the synthesis parameters of porous silicate materials prepared by sol-gel and template methods

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Silica gels with defined porous structure are widely used in industry. In general, synthesis of silica gels consists of three main stages: hydrolysis of silica (the silica alkoxides are used as a source of silica), gelling and drying. Template method supposes the addition of the organic substances before gelling of sol and using the calcination as the last step. The 16 samples of porous silicate materials were prepared at different conditions. For each sample, two alkoxides were used simultaneously. The template agent was phenol. The varied factors were ratio of alkoxides, presence of template agent, dilution of sol by solvent before gelling and alkoxide types. The nitrogen adsorption/desorption isotherms were measured at -196 °C using volumetric apparatus Nova 1200e Quantachrome. The specific surface area (S) was obtained using the BET method (using desorption data), volume micropores (Vmicro) – from t-plots, summary pore volume (Vs) was obtained at P/P0=0.95. Pore size (d) was calculated by BJH method for all samples. The influence of factors on final porous structure was estimated by ANOVA method. The effects of factors were found and optimal conditions were proposed.

[609]

Strategic Development of Fischer-Tropsch Process based on Economic and Technological Feasibilities

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Fischer-Tropsch(F-T) synthesis technology was developed to convert fuel feedstock such as natural gas and coal into transportation fuels and heavy hydrocarbons. Despite constant research activities on this technology in recent years, there is still scope for research and development especially about strategic development of F-T process, which considers both economic and technological feasibilities.

The aim of this study was to optimize F-T plants to procduce gasoline and gas oil by investigating the benefits of recycling & co-feeding of unconverted gas, undesired compounds, and lighter hydrocarbons into a reactor and minimizing capital and operating costs. This research involved the development of F-T reaction system. For this, both two-phase and three-phase reactor models were developed, and the results of each reactor model were compared each other. The kinetic parameters for these models were estimated using MATLAB fitting to experimental data, and these models were then applied to ASPEN HYSYS flowsheets to simulate various F-T plant design configurations. The results showed that the recycling and co-feeding to F-T reactor plant is beneficial for the production of gasoline and gas oil with high efficiency.

[617]

A thermodynamic targeting approach for the synthesis of sustainable biorefineries

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One of the major challenges of achieving a sustainable integrated bio-refinery lies in the systematic synthesis and design of such systems. Biorefineries are complex systems, involving many processes with many parameters and constraints.The feedstock to the process can be diverse and a multitude of products can be produced. There is a need to develop quick and efficient methods to screen the variousproduct options in order to determine which products best utilise thefeedstock. The other key aim is to improve the efficiency, economics and reducethe environmental impact of such processes. This contribution develops upfront conceptual-level design targets, based onfundamental concepts such as mass conservation, energy conservation and thesecond law of thermodynamics, for the production of fuels (such as ethanoland hydrocarbons) and chemicals (such as hydrogen and methanol) from biomass. These targets aim to provide insight into the design of sustainable biorefineries, prior to the detailed design, with an aim of maximising feedstock utilisation thereby increasing the process efficiency and reducing the emissions from such processes. The targets for these different products are compared using sustainability metrics such atom economy and E-factors. Products which maximise the atom economy are determined. This work will further identify integration opportunities and assess whether combining the production of fuels andchemicals, as well the utilisation of hybrid feedstocks can achieve higher process efficiencies.

[619]

Formulation of a Network and the Study of Reaction Paths for the Sustainable Reduction of CO2 Emissions

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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. Carbon dioxide (CO_2) is the largest source and the reduction of the amount emitted is primary focus of developments. A new and promising process that reduces the emissions is the conversion of CO_2 into useful products, such as methanol and dimethyl carbonate (DMC) [1]. In this work, through a computer-aided framework for process network synthesis-design, a network of conversion processes that all use emitted CO_2 is investigated. The methodology being developed involves the formulation of a superstructure-based network of CO2 conversion processes.

From reviews of work previously done, there are ranges of possible products that are formed directly from CO_2 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 CO_2 utilization to a variety of products. Each of the paths in the network involves CO_2 and a co-reactant, such as hydrogen, reacting to produce various chemical products, such as methanol and dimethyl ether. The process network evolves as some of the reactions involve products from other reactions as a reactant. This yields a network of products that can be created using only the CO_2 emissions and not adding any CO_2 emissions through the reactions.

With the use of computer-aided tools, this network, and the information contained within it, is generated. The detailed simulations, of CO_2 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 CO_2 and other greenhouse gases, and creating more energy efficient processes.

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[623]

A Sustainability Driven Methodology for Process Synthesis in Agro-Food Industry

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Within the agro-food industry, agro-materials are converted into a range of valuable semi-finished and finished products. To reach a sustainable, resource efficient food system, the optimal process pathways converting the agro-material into these products have to be identified. To identify these pathways, a systematic Process Synthesis (PS) method is needed for the agro-food industry. This sustainability driven PS method should enable the synthesis of the optimal process pathways, converting an agro-material into a range of valuable products, producing minimal waste or low-value by-products. In this paper, the elements required for such a method are proposed. The relevance of these elements is illustrated with a simple illustrative case for the processing of tropical fruit. The proposed approach uses Multi-Objective Optimisation methods, to provide decision support for PS to decision makers in the agro-food industry. This leads to new insights in optimal pathways for processing agro-materials for the agro-food industry.

[629]

Integrated Design of Working Fluid, Process and Turbine of Organic Rankine Cycles using PC-SAFT

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Optimal performance of an Organic Rankine Cycle (ORC) requires both working fluid selection and process optimization. Today, these problems are typically tackled in a two-step approach: working fluid candidates are pre-selected first and the corresponding process is optimized in a second step. If the criteria for the preselection fail, suboptimal solutions are obtained. Simultaneous optimization of working fluid and process is therefore desirable but leads to a mixed-integer nonlinear program (MINLP) of prohibitive size and complexity. To circumvent this problem, the authors recently proposed a computer-aided molecular design (CAMD) framework for ORC working fluids [1,2]. Here, the working fluid is modelled using the PC-SAFT [3] equation of state. The discrete pure component parameters representing the working fluid are optimized simultaneously with the process by relaxation in the continuous-molecular targeting (CoMT) step. Since the relaxed optimal working fluid parameters will not coincide with any real working fluid, a mapping step identifies real working fluids.

While the CoMT-CAMD framework achieved a close integration of fluid and process, the technology models employed have still been simple. In particular, constant efficiencies were assumed for the turbine independent of the chosen fluid. This assumption is common practice in working fluid selection despite the interdependence of the working fluid and turbine performance.

In this work, we integrated a preliminary design model for the radial turbine of the ORC in the CoMT-CAMD framework. The design model estimates the efficiency of the turbine and its key design parameters. Constraints are set on the critical design parameters (e.g., blade height, speed of rotation, volume ratio, or Mach number). Thereby, working fluids can be identified which lead to suboptimal turbine efficiency or even infeasible turbine designs.

The mapping step is performed by CAMD using a recently developed design group-contribution method for PC-SAFT [2]. The objective of the CAMD mapping is to design working fluids with performance as close as possible to the hypothetical optimal working fluid. The performance of the designed molecular structures is directly calculated from the pure component parameters using a Taylor approximation of the process objective function. The framework is demonstrated in a case study. A small scale solar power cycle is optimized and a working fluid is selected enabling the design of an efficient radial inflow turbine. The influence of the turbine design on the optimal solution is shown.

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[637]

Evaluation of Dimethyl Carbonate and Ethylene Glycol Production from Biomass

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In this study, a process for production of dimethyl carbonate (DMC) and ethylene glycol (EG) from biomass is proposed. The process starts with biomass gasification to obtain synthesis gas with a composition suitable for synthesis of methanol (MeOH). CO2 in the synthesis gas is removed in a bed of CaO for further utilization for ethylene carbonate (EC) production from ethylene oxide and CO2. Then MeOH and EC undergo transesterification to DMC and EG in a reactive distillation connected with an extractive distillation. The effects of key operating parameters of different units were determined using ASPEN PLUS simulator to find their suitable operating conditions. The process design was based on the product purities of 99.5% (for each of DMC and EG) and the energy self-sufficient condition. Biomass combustion was the main source of energy generation for the system. The process was further improved by implementing the concept of heat exchanger network. It was found that the atom efficiencies of the process with heat exchanger network indicate higher values (C: 37.80, H: 55.23, O: 41.45) than those of the process without heat exchanger network (C: 32.87, H: 48.96, O: 37.72) since less biomass is required for heat generation and therefore it is more effectively converted to DMC and EG. The energy consumptions were reported by allocating to both desired products as 13.97 MJ/kg-DMC and 9.63MJ/kg-EG. Since all energy was supplied by biomass itself, the process was considered as carbon neutral with a fraction of carbon dioxide fixation from biomass into chemicals of 0.28.

[647]

Topology optimization for biocatalytic microreactor configurations

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Nowadays, there are several methods for the immobilization of enzymes such as on solid or porous supports, entrapment in polymeric matrices and cross-linking. This project consists of a computational study of a novel way for enzyme immobilization.

γ-Prefoldin is a molecular chaperone with a filamentous protein structure discovered from the hyperthermophile Methanocaldococcus jannaschi. Genetic modification allows filaments generation with different length. The filaments length can vary from 200 nm up to 2 μm in length.

In addition, the development of protein connectors which are able to link filaments can expand the nanowires into 2 or 3 dimensional structures. In the literature, two types of connectors have been described: 2 way connectors which permit the construction of 2D self-closing structures and 3 way connectors which can develop into complex 3D structures. One possible application for filamentous protein molecules is the enzyme immobilization on their surfaces.

The formation of controllable size 2D and 3D shapes from stable protein filaments combined with the opportunity for immobilization of enzymes constitute the motivation to investigate and optimize the distribution of immobilized enzyme for improvement of the space-time yield.

This study investigates the distribution of two enzymes for a multi-enzyme system immobilized on a filamentous nanowire structure of γ-prefoldin (γ-PFD). The multi-enzyme system will be chosen before starting the investigation. Examples of multi-enzyme systems are glucose oxidase and catalase system, and the transaminase and alanine dehydrogenase system.

This work includes a routine which will implement kinetic models into a CFD framework (Ansys CFX®) which will be coupled with a Matlab® routine performing the optimization by making changes to enzymes distribution and running the simulation for each new enzyme distribution. At last, the performance of the system is evaluated by an objective function, and the optimization procedure will be established by an evolutionary optimization.

This project will allow the generation of optimal immobilized enzyme configurations and afterwards studying it in the laboratory. Therefore, this approach is useful to understand enzymatic reaction systems as well as to investigate and develop new strategies for reactors for the pharmaceutical industry.

[656]

Development of New Generations of Synthetic Fuels and Value-added Chemicals from Natural Gas via GTL

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This paper summarizes our research activities at Texas A&M University at Qatar during the past six years in the advancement of synthetic fuels and value-added chemicals obtained from natural gas via gas-to-liquid (GTL) technology, an area which is of key economic importance to the state of Qatar. Despite similarity in carbon number composition, fuels obtained from crude oil differ greatly in terms of chemical structure from those obtained via XTL (X-to-liquid) processes, which involve the conversion of synthesis gas (CO + H2) derived from natural gas, coal or biomass. Bringing GTL products to market therefore requires an in-depth knowledge of the composition and properties of synthetic fuels to design new and efficient formulations of these products. Our initial efforts in this area started with a project to boost Shell's aviation fuels obtained from its world leading Pearl GTL plant in Qatar. Currently, we are building on our previous work in collaboration with the Technical University of Denmark (DTU) and Texas A&M University at College Station, and are supported by industry partners such as General Electric (GE Oil & Gas) and Oryx GTL (a joint venture between Sasol and Qatar Petroleum). During the first phase of our aviation fuel project in collaboration with Shell, Rolls Royce, University of Sheffield, and DLR (the German Aerospace Institution) we built a sophisticated fuel characterization laboratory. We prepared model fuel blends composed of n-, iso- and cyclic-paraffins to represent synthetic paraffinic kerosene (SPK) in order to investigate the effect of fuel functional group composition on the properties. For this purpose, we carried out a systematic experimental campaign coupled with sophisticated statistical and visualization analysis using artificial neural network (ANN) and multiple linear regression (MLR) models to develop composition-property correlations. This approach helped us to identify optimum compositions for the synthetic aviation fuels that meet aviation industry standards for certification [1]. In the second phase of the project we investigated to include the role of aromatics on enhancing critical properties such as the density, lubricity and elastomer compatibility of aviation fuels, by preparing a series of SPK blends with different additives (e.g. ShellSol A150, toluene and styrene) and measuring certain key physical properties such as density, heat content, freezing point, flash point, vapour pressure, and viscosity. This campaign will be extended in future to investigate the possibility of replacing the aromatics (that are known of their negative environmental impact) with heavy paraffinic hydrocarbons. As part of our collaboration with DTU we are providing experimental data to validate predictive models developed at the Computer Aided Process Engineering Centre (CAPEC) which will greatly reduce the amount of time and resources needed to formulate fuel blends with certain desired properties by eliminating the need for laboratory testing. Another current project being undertaken in our lab is focused on the fractional distillation of synthetic fuels into different boiling range cuts in order to study the carbon number effect on the blend properties. This work will be used to identify potential value-added products from Qatar's synthetic crude stream from the Oryx GTL plant in Qatar.

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[688]

Design of Hybrid Heat-integrated Configuration for Indirect Reactive Distillation Processes

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In this work, hybrid configuration which combines the concepts of thermally coupled and multi-effect heat-integrated methods has been studied. Moreover, the potential energy saving of other individual heat-integrated methods has been compared with the hybrid configuration. Ideal IIp reactive distillation process and diphenyl carbonate process are chosen as examples to demonstrate the performance of the hybrid configuration. The result shows hybrid configuration displays the highest ability in energy saving for both processes.

[696]

Simulation of carbon-dioxide-capture process using aqueous ammonia

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Nowadays, the release of carbon dioxide (CO2) becomes an issue for many industry due to global warming effects especially coal-fired power plant. Aqueous ammonia process is a promising way to be used instead of conventional CO2 capture process using monoethanolamine (MEA) in post-combustion CO2 capture. Ammonia-based CO2 capture process simulation has been developed by Aspen Plus and validated with case study from literatures. Simulation process consists of two parts; CO2 absorption process and ammonia abatement process. The simulation process was developed to satisfy operating condition target of 90% CO2 recovery and improved by using heat integration to minimize energy requirement. The result showed that the performance of aqueous ammonia process provides more efficiency in term of energy requirement for absorbent regeneration and investment cost, based on standard environmental regulations, compared to MEA based process.

[710]

Energy efficient bioethanol purification by heat pump assisted extractive distillation in a dividing-wall column

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The industrial production of bioethanol fuel requires energy demanding separation steps to concentrate the diluted streams from the fermentation stage and to overcome the azeotropic behavior of the ethanol-water mixture. The classis separation sequence consists of three distillation columns performing several tasks penalized by high energy requirements: pre-concentration of ethanol, extractive distillation and solvent recovery.[1,2]

A previous study proposed the use of an extractive dividing-wall column (E-DWC) that combines the extractive distillation column (EDC) and the solvent recovery column (SRC) of the classic sequence into one unit.[3] In a follow-up study, the E-DWC configuration was extended to include also the pre-concentration distillation column (PDC) thus being able to concentrate and dehydrate bioethanol in just a single step.[4]

In this work, we consider a vapor recompression (VRC) heat-pump-assisted E-DWC, in which the ethanol top vapor stream of the E-DWC is recompressed from atmospheric pressure up to 3.7 bar (thus to a higher temperature) and used to drive the side reboiler responsible for water vaporization. A mixture of 10%wt ethanol (100 ktpy plant) was considered to be concentrated and dehydrated using ethylene glycol as mass separating agent. Rigorous simulations and optimization of the vapor recompression assisted E-DWC were carried out in Aspen Plus.

The results show that the energy requirements drop from 2.07 kW.h/kg (classic sequence) to only 1.24 kW.h/kg ethanol for the VRC-E-DWC system, thus energy savings of 40% being possible. However, considering the requirements for a compressor and use of electricity in case of the heat pump assisted alternative, the annual costs are reduced by 24% in case of the novel VRC-E-DWC alternative, as compared to the conventional separation process.

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[713]

Optimal design and plantwide control of di-n-pentyl ether processes

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Di-n-pentyl ether (DNPE) is an excellent candidate for diesel fuel formulations because of its blending cetane number, good cold flow properties and effectiveness in reducing diesel exhaust emissions, particulates and smokes. Moreover, 1-butene is an appropriate feedstock for DNPE production, as it can be selectively hydroformylated and hydrogenated to 1-pentanol. As reported in literature, thermally stable resins such as Amberlyst 70 are excellent catalysts for 1-pentanol dehydration, having high activity and selectivity at temperatures up to 463 K.

1-Pentanol dehydration is slightly endothermic and can be performed in an adiabatic reactor. However, because the reaction is equilibrium limited, complete reactant conversion is not possible. Therefore, reactant separation and recycle are necessary. Alternatively, equilibrium displacement can be achieved by removing at least one product from the reaction mixture. The use of a membrane reactor was suggested as an option for in-situ water removal. Although high reactant conversion is possible, this option is plagued by the high cost and the reduced service life of the membrane. Moreover, one distillation unit is still necessary for the separation of 1-pentanol and DNPE. As a result, the unit cost of the DNPE product is rather high (1.6 US$/L).

In this contribution, we propose and investigate two alternative options for DNPE production. In a conventional plant, the reaction takes place in an adiabatic tubular reactor. From the reactor effluent, the heterogeneous water / 1-pentanol azeotrope is obtained as distillate in a first distillation step. After decanting, water product is obtained at a purity exceeding 99.7 %, while the organic phase is refluxed. The bottom product is sent to the second distillation column where the DNPE product (over 99.9% purity) and the 1-pentanol recycle are obtained. In the second alternative process, catalytic distillation is used to perform both reaction and separation in the same unit. The reactant is fed at the top of the reactive section. High purity (over 99.9%) DNPE is obtained as bottom product, while the vapor distillate is condensed and sent to liquid-liquid separation, which gives the product water product and the organic reflux.

For each alternative, the key design decisions are identified and steady state optimization is performed in Aspen Plus. Optimization was performed using Differential Evolution with Taboo List (DETL), by coupling Aspen Plus with Matlab. The objective function and decision variables are the total annual cost (TAC) and variables such as reactor size, distillation number of trays, reflux ratio, feed location, and tray catalyst loading. The process alternatives are analyzed in terms of energy requirements, total investment, operating and annual costs. Finally, the controllability is assessed by rigorous dynamic simulation performed in Aspen Dynamics. The conclusion is that compared to the membrane reactor alternative, both alternatives (conventional reaction-separation-recycle process and the compact catalytic distillation) are better DNPE process candidates, requiring simpler units leading to much smaller investment costs and reduced energy requirements (only 655 kWh/ton DNPE), while also having good controllability.

[716]

Process Design of a Multi-Product Lignocellulosic Biorefinery

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Second generation biorefineries are considered promising processes in order to convert lignocellulosic biomass not only to biofuels for transportation, but also to added-value chemicals.

Several alternative process pathways including biochemical and thermochemical conversions are available. In this view the conceptual design of a superstructure and optimization methods for process synthesis are widely used in order to find the optimal process flowsheet (Stefanakis et al., 2014).

A previous work (Giuliano et al., 2014) addressed the construction of a superstructure for a multi-product lignocellulosic biorefinery producing levulinic acid, succinic acid and ethanol. Mixed integer linear programming (MILP) was used to find the optimal solution in terms of process flowsheet and biomass allocation. The economic objective function was based on the net present value (NPV) of the biorefinery production. The objective function value was subject to approximations arising from the use of approximated methods for the sizing of the equipments and from the linearization of the nonlinear problem.

In the present work the flowsheet resulting from the optimization of the lignocellulosic biorefinery superstructure was simulated by a process simulator (Aspen Plus). As a result, rigorous methods were used to calculate values of the stream thermodynamic properties and to model the process units. Therefore, process simulations provided more precise values of the process yields and of the equipment size with respect to those obtained with the MILP analysis. Economic analysis was applied to assess the economic feasibility of the process. Sensitivity analysis on the size of the plant, the product prices, the biomass price was carried out as well. The economic results obtained with the process simulations were compared with those obtained with the mathematical programming to assess the influence of the linear approximation on the process optimization.

Future work will consist in updating the process conditions and yields and unit sizes obtained by process simulations into the superstructure. An iterative procedure coupling MILP method and process simulation will be proposed.

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[732]

MINLP optimization model for water/wastewater networks with multiple contaminants

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Water is the main resources for process industry both direct and indirect usages. The reduction of water usage decreases the capital cost for process industry. This paper presents a method minimizing water usage in water/wastewater network with multiple contaminants by generating water and waste water treatment networks. It includes two steps of calculations. The first step is initialization step with non-linear programming (NLP) for generating the topology of minimum water flowrate network and the second step is optimizing step with mixed-integer non-linear programming (MINLP) for minimizing fresh water in water flowrate network. The main objective of this model is minimizing water usage and wastewater in water/wastewater network. This model uses data as the case study from the literatures of Débora C. Faria et al. (2008). All mathematical models of this work are a solved by DICOPT as solver of General Algebraic Modelling System (GAMS).

[740]

Design of Separation Processes with Ionic Liquids

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One of several challenging problems in the petrochemical and chemical fields is a separation of both aqueous and non-aqueous systems involving with azeotropic, close-boiling and low relative volatility mixtures. Extractive distillation is a common and efficient separation process involving an addition of a heavy component, namely entrainer, which is completely miscible with the target solute component in an azeotropic mixture. Ionic liquids (ILs) have recently become alternative entrainers due to their outstanding structures and properties including stability, non-volatility and others related to environmental concern. The systematic methodology of selecting the suitable ionic liquids as entrainers in the extractive distillation can be accomplished by using a computer-aided molecular design (CAMD). The predictive thermodynamic property model is the important parameter for the screening of ILs as entrainers. The Hildebrand solubility parameter Group Contribution along with the miscibility from experimental data collected from literature are used as a tool to screen suitable IL entrainers in the aqueous azeotropic systems (e.g. ethanol + water and isopropanol). Furthermore, it is aimed to demonstrate the proposed methodology to screen suitable ILs as entrainers in more complex non-aqueous azeotropic systems, for instance, alcohol + aliphatic hydrocarbons, aromatic + aliphatic hydrocarbons and aromatic + cyclic hydrocarbons. The vapor-liquid equilibrium are then constructed by using the binary parameter NRTL model via ICAS program in order to determine the minimum IL concentration and to confirm the breaking of azeotropes. Finally an economic evaluation of the best IL entrainer is analyzed in term of their energy consumption as compared to the conventional organic solvents by using the PROII program.

[746]

New synthesis framework for the optimization of multicomponent gas membrane separation systems

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During the last 20 years, membrane technology has evolved from a laboratory tool to reliable industrial products. Due to the constantly improving materials and preparation methods, a variety of high performance membranes have emerged and been employed successfully in industrial gas separation. A majority of the researches available in the literature were focused on the modeling, simulation and optimization of gas separation systems with a single specified membrane (Tessendorf, Gani & Michelsen, 1999, Chem. Eng. Sci., 54: 943.). But how to optimally design a gas separation system which can separate a mixture containing three or more components into three or more product streams. Only a few method have been proposed to address this problem.

The pioneering work was done by Agrawal (Agrawal, 1996, Ind. Eng. Chem. Res., 35: 3607.), who drew the n-component gas separation membrane cascade superstructures by simple analogy with distillation schemes. However, components are arranged in the order of increasing boiling point in distillation sequence synthesis, which does not apply to the membrane systems. The membrane separation sequences and cut ratios are only dependent on the membrane used, which means the theoretical combinations of the membrane separation sequences are much more than that of the corresponding distillation sequences.

Besides membrane separation sequences, the choice of the membrane is another important decision to make, because various membranes with different performances (selectivity, flux and operating conditions) and prices are available to fulfill the same separation task. In the previous literature, membrane used is predefined based on human insights before the optimization of the whole system. So the tradeoff between performance and capital investment and the advantage of the combinations of different membranes are not included in those approaches.

Based on these considerations above, A hierarchical conceptual design framework consists of three stages is introduced to synthesize the optimal multicomponent gas membrane separation systems. In stage 1, a state-task-network derived from the information of candidate membranes is introduced to realize the separation feasibility analysis. In stage 2, a new state space superstructure based on Generalized Membrane Stage (GMS), which is inspired by Generalized Modular Framework (Proios & Pistikopoulos, 2006, AIChE J., 2006, 52: 1038.) and Mass–Energy Stage (Zou, Cui, Dong, Wang & Grossmann, 2012, Chem. Eng. Sci., 2012, 75: 133.), is proposed to represent all feasible substructures with minimum redundancy. The corresponding MINLP model advocates the use of short-cut design formulations. In stage 3, An MINLP design model is developed to minimize the total annual cost by simultaneous optimization of the permeator configurations and operating conditions in each GMS. The rigorous permeator model is adopted to ensure practical reliability and optimality of the attained designs (Qi & Henson. 2000, Comp. Chem. Eng., 24: 2719.). Finally, a refinery off-gas separation case is presented to illustrate the proposed framework.

[755]

Systematic Screening of Fermentation Products as Future Platform Chemicals for Biofuels

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The envisioned raw material change from a fossil- towards a bio-based industry will lead to new platform chemicals [1] and products and offers the chance to realize alternative processing concepts. In the case of second generation biofuels, the competition with the existing fossil-based fuels is a major challenge. Research and development has to focus on the most promising products and process alternatives, which requires identification of these pathways from lignocellulosic biomass to biofuel candidates using scarce data of high uncertainty. A recent ranking of possible biofuels by fermentation considered the productivity of the fermentation to estimate process performance [2]. A more rigorous screening of possible pathways can be carried out by the optimization-based Reaction Network Flux Analysis (RNFA) utilizing reaction stoichiometry, reaction yields, enthalpy-cost correlations and a first assessment of the environmental impact [3].

Herein, RNFA is extended to include the calculation of the process energy demand, equipment costs and the environmental impact of the overall process. Different fermentations as well as various downstream processing concepts are then analyzed according to their energy requirement, total annualized costs (TAC) and environmental impact of processing (EIP), i.e., global warming potential and toxicity potential. The first step is an evaluation based on the theoretical and achievable fermentation yield, productivity and titer, which are either literature known or easily accessible by first laboratory experiments. In a second step the analysis includes the downstream processing to rank the process performance of fermentative products as platform chemicals for biofuels.

The analysis of fermentation shows the tradeoff between maximizing the yield and the productivity in both the TAC and EIP. While a low yield leads to an increase in the raw material costs and determines the CO2 uptake or release during fermentation, a low productivity causes high investment costs as well as a high energy requirement and enhanced emissions. The resulting energy demand is further increased considering the downstream processing rendering low fermentation concentrations inefficient. Finally, the production of platform chemicals is benchmarked to state of the art fuels like gasoline revealing performance targets for the fermentation research. By extending the methodology, a more detailed and meaningful screening of fermentative platform chemicals is possible.

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[758]

Design of an Integrated Process based on Chemical Sequestration of CO2 from a Power Plant

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Global economic development has anticipated the growth on demand of the energy sector whose supply in the coming decades will still remain achieved by burning fossil fuels. The needs to stabilize the CO2 atmospheric concentration require technologies for capturing and reutilization of this greenhouse gas. Such scenario motivates feasibility analysis of power generation with post-combustion capture of CO2 from the flue gas associated with its transformation into chemical commodities. Specifically, the economic performance of an integrated process for CO2 capture and conversion to chemicals is evaluated in order to balance revenues and energy penalty. The study uses CO2 capture with MEA (monoethanolamine), including compression of the captured gas followed by its conversion to chemicals. The focus is the design of an integrated process for the production of methanol (MeOH), organic carbonates (dimethyl carbonate (DMC), diethyl carbonate (DEC), propylene carbonate), olefins (ethylene and propylene) and ethylene oxide (EO). However, kinetic and thermodynamic stability of CO2 molecule present significant challenges in designing efficient chemical transformations based on its potential as feedstock. Most important challenge is that of the catalyst. In this sense, specific catalysts have been synthetized in order to achieve suitable conversion and selectivity to make the processes economically feasible. The analysis includes definition of project assumptions, followed by design of the process flowsheet for different scenarios, process simulation and sizing of the main process equipment for economic analysis - capital and operational expenditures (CAPEX and OPEX). In the methodology used, process simulation and optimization were employed to compare process performances at maximum yields. Technical indexes for each process were analyzed based on revenues and energy requirements in a specific range of production capacity of each chemical produced. Economic optimization was carried out for the alternative routes aiming to maximize annual profit (US$/year) in order to make process profitable and achieve the desired environmental remediation. Preliminary results have shown that the lowest rate of CO2 emission is achieved for ethylene oxide production process, considering thermal and electrical consumption of 13kt/year and 597 t/year, respectively. However, all processes have great potential concerning CO2 chemical sequestration through it conversion to higher value products. The final results are expected to show indexes for technical and economic performance of the integrated flowsheet in the optimal process conditions in order to achieve process viability.

[761]

From Fed-Batch to Continuous Enzymatic Biodiesel Production

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Industrially, the enzymatic production of biodiesel is performed via fed-batch operation so as to minimize the inhibition and deactivation of the biocatalyst. Operating in Fed-batch has proven reliable in terms of practical operation. However, the main disadvantage is the downtime between batches.

To guide process development of a continuous enzymatic biodiesel process, a mechanistic model of the process is developed which moves beyond the use of levenspiel plots to determine reactor residence times for a desired conversion. The drawback with a detailed mechanistic model is that given the large number of parameters and the often few experimental data points, the parameters found are not identifiable. The model is then only applicable within the operating range for which the model was validated. We hypothesise that by fitting this model to fed-batch and continuous stirred tank reactor (CSTR) data, it will enable us to use the model for determination of residence times to reach a specified conversion in a CSTR. This unique approach fits the validation dataset for the five measured components (triglycerides, diglycerides, monoglycerides, free fatty acid and fatty acid methyl esters (biodiesel)) much better than using fed-batch data alone.

The model is then used to predict that 5 reactors will be needed with a combined residence time of 28 hours to give comparable performance to a fed-batch operation which lasts 24 hrs. The simulations show that in one month the CSTR process is able to process 4% more oil compared to fed-batch operations, assuming a 6 hour emptying and filling time for the fed-batch reaction.

[775]

Feed Flexibility of CH4 Combined Reforming for Methanol Production

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Natural gas with high CO2 content is a highly available resource, whose application for synthesis gas (syngas) production through dry reforming is strictly limited to processes that require low H2/CO ratios. In a recent work we have stated that methanol production through a process scheme based on the combined reforming (CO2+H2O) of methane becomes a viable alternative from both technical and economic points of view. A membrane H2 separation unit and partial H2 reinjection have been considered for the adjustment of syngas composition to stoichiometric conditions. Both the methanol synthesis reactor and the reformer operate at thermodynamic equilibrium conditions, i.e. at 250°C and 71 bar for the former, and at 950°C and 20 bar for the latter. These conditions are customary at industrial practice. In the reformer, a natural gas containing 30% CO2 with H2O/CH4 = 2 has been adopted. CO2/CO ratio and CO2 concentration at the methanol reactor inlet were also restricted to those values commonly employed at industrial practice, since a high CO2 content might have a negative effect over methanol production rate and catalyst stability. We have assessed that, under the above mentioned operating conditions, the employment of combined reforming for methanol synthesis turns out to be economically advantageous over the classical steam reforming process.

In this work a study of the feed flexibility for combined reforming is developed, by taking into account the existence of fields with CO2 contents higher than 30%. A higher CO2 content in the feed gas implies a syngas with a lower H2/(CO+CO2) ratio, which forces an increase in the H2 separation and reinjection rates. This situation has a negative effect on the reformer's energy balance and consequently, on process economy. Partial separation of CO2 from the raw syngas might be necessary downstream the methanol reactor, in case CO2 content were extremely high, this way increasing process complexity and cost. It is shown that on the basis of a natural gas with 30% CO2 content, processing one with a higher content brings about the following features: a higher natural gas consumption as fuel to the reformer, a higher H2 separation and a lower recycle ratio, apart from requiring a partial CO2 removal. It should be noted that a 15% increase in H2O/CH4 ratio has little effect over the process.

[831]

Simultaneous optimization approach for integrated batch water-allocation and heat exchange network

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In recently years, integrated optimization of energy and water use in batch process draws more attention. Halim and Srinivasan firstly (Comp. Chem. Eng., 2011, 35: 1575.) proposed a sequential methodology, in which it contains one optimal schedule main problem and two network sub problems (heat integration/water reuse), to deal with this issue. Furthermore, Majozi and coworkers(Ind. Eng. Chem. Res., 2013, 52:8488) proposed a unified framework to simultaneously optimize both water and energy usage with flexible schedules, in which the heat storage is introduced to utilize the heat energy at different time slot. They also introduce the time average model (TAM) and time slice model (TSM) (Chem. Eng. Sci., 2014, 111:335) into synthesis system to keep the flexibility of the schedule and narrow the gap of simultaneously solving energy integration and wastewater minimization problem in the same scheduling framework. However, there are still two main limitations in their framework. Firstly, only washing operation is considered in the optimization of multipurpose batch plant which may contain water consuming/generating reactions and water treatment operations. Secondly, heat exchange between water streams in water allocation network is not considered so that a more practical heat exchange network cannot be obtained.

In this paper, a systematic methodology is developed to deal with the simultaneous optimization of water-allocation network and heat exchange network (WAHEN) in multipurpose batch plants under undetermined schedule. Based on the WAHEN (Chem. Eng. Sci., 2008, 63:3664; Ind. Eng. Chem. Res., 2012, 51:4299; Ind. Eng. Chem. Res., 2012, 51: 14793). and batch water allocation network (Comp. Chem. Eng., 2009, 33:1153; Ind. Eng. Chem. Res., 2010, 49:236), we modified the State Space WAHEN superstructure to a State Time Space WAHEN superstructure which contains the distribution network (DN) block, process operation (PO) block and time axis. The PO block contains WAN sub-block and HEN sub-block separately. The HEN sub-block is introduced not only to fulfill heat exchange task between units but also to cover all the stream match combinations. WAN sub-block is introduced to deal with three types of water operations (water consuming/generating/treatment). Besides, a time axis is introduced to indicate the starting and finishing time of a task.

Then, we formulate a MINLP model which contains batch process schedule sub-model, WAN sub-model, and HEN sub-model. It should be noted that a logic pre-analysis is performed to testify the possible combinations of binary variables which indicate the connection relationship between heat generating/consuming unit.

Due to the scale of the problem and the nature of MINLP, we proposed a stochastic solution strategy which contains 3 steps. The first step is to generate a set of initial guesses of the determined variables randomly. The second step is to use the initial value we generated to obtain the candidate feasible solutions in GAMS with DICOPT. And the final step is to obtain the better solution by shifting the value of some binary variables. For some extra large scale cases, a heuristic algorithm like GA/SA can also be considered.

[854]

Process alternatives for second generation ethanol production from sugarcane bagasse

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The production of ethanol from sugarcane juice in Brazil is already an established process. In an autonomous distillery, sugarcane juice is extracted, treated to eliminate possible inhibitors and fermented by Saccharomyces cerevisiae to ethanol. The alcoholic solution is purified and fuel ethanol, both hydrous and anhydrous, can be produced. Sugarcane bagasse, on the other hand, is burned in a combined heat and power (CHP) stage to meet the steam and electric energy demand for the ethanol recovery process. Nevertheless, a surplus of bagasse is frequently possible and this opens opportunities to produce and sell electric energy to the grid or alternatively to increase ethanol yields through second generation ethanol production. While the feasibility of the production of electrical energy is very well assessed, there are uncertainties about second generation ethanol, both from technical and economic viewpoints. Thus, a rigorous consideration of the economic metrics of this process is important to identify the bottlenecks of the system and find possible solutions.

The process considered is this work for second generation ethanol production involves liquid hot water pretreatment of sugarcane bagasse, followed by enzymatic hydrolysis. The solid fraction is hydrolyzed and the glucose liquor produced is subsequently fermented by S. cerevisiae. These steps can be performed separately or in the same reactor (Simultaneous Saccharification and Fermentation, SSF). The liquid fraction, which consists mainly of xylose from the hemicellulose hydrolysis is also fermented, increasing ethanol production. Both alcoholic solutions are filtered to separate the solids consisting of non-hydrolyzed cellulose, lignin and yeast cells. These solids are separated and sent to the CHP stage, while the liquid fraction is sent to distillation to recover hydrous ethanol.

The production of low added-value chemicals, such as fuel ethanol, imposes challenges in the design of the process, since the profit margins are usually low. In this context, this study simulated a second generation ethanol production plant using experimental data for the reaction steps. The simulations were used to assess the main operating and capital costs of the process and analyze the impact of the process metrics on them. Finally, based on general information about the inhibitory effects on the hydrolysis and fermentation reactions, some alternatives are sought to improve the process. The analysis shows that the hydrolysis step is still the main bottleneck of the process, which is mainly due to the low space-time and biocatalyst yields in the reactor.

[859]

Method for innovative synthesis-design of chemical process flowsheets

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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, mathematical programming, hybrid, etc.) have been proposed and are also currently employed to solve these synthesis-design problems. D' Anterroches [1] 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 [2]. 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. The implemented framework in the form of a new computer-aided tool in ICAS (Integrated Computer Aided System) will be highlighted through two case studies, one involving the synthesis of a chemical process flowsheet (the well-known Hydrodealkylation of toluene process) and another for a biochemical process flowsheet (production of ethanol from lignocellulose). In both cases, not only the reported designs are found and matched, but also new innovative designs are found, which is possible because of the predictive nature of the models.

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.

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[866]

Simulation study of heat transfer enhancement due to wall boiling condition in a microchannel reactor block for Fischer-Tropsch synthesis

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A reactor for Fischer-Tropsch(FT) synthesis involves substantial heat effect due to high exothermic nature of FT- reacion. In this work, Computational Fluid Dyanmic (CFD) simulation of heat transfer in the microchannel block for FT synthesis is studied to gain insights on the thermal behavior of a compact reactor block and optimize the reactor performance in terms of thermal control. The microchannel reactor block consist of alternate process channel and coolant channel planes. Catalyst filled process channels are modeled as pack-bed reactor and the source for heat generation; and coolant channel as heat sinks. Cooling oil, saturated liquid water, subcooled liquid water and superheated vapor were chosen to simulate the single phase and multiphase coolant flow simulation. Heat transfer enhancement due to wall boiling condition (heat transfer invloving phase change), as comapred to the case that do not invlove phase change was evaluated. Average heat flux under wall boiling condition was 1 to 2 order higher than of the cases that do not have wall boiling condition, implying wall boiling significantly enhance the heat transfer across the microchannel walls. Scenerios for for partial and complete boiling, with saturated water as coolant, was investigated. Simulation study was carried out for a range of operable values of syn-gas flowrates and coolant flowrates to explore the feasible operating range.

[880]

Optimization of the Integrated Gasification Combined Cycle using Advanced Mathematical Models

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Integrated Gasification Combined Cycle (IGCC) is a prefered technology to increase efficiency and reduce environmental emissions associated with fossil fuel. Several simulation models to study the performance of an IGCC power plant, particularly focusing on the gasification unit, have been developed and published in open literature. These range from a simple 1-Dimensional model to complex 2-D and 3-D Computational Fluid Dynamics (CFD) models. The Entrained Flow Coal Gasifier (EFG) which is commonly used in IGCC is known to operate under severe operating conditions, up to 2000oC and 8.0 MPa. While the EFG achieves very high conversions, up to 99%, the extreme conditions impact negatively on the capital investment of the gasifier and the downstream units. Published models have however not proven if the extreme conditions are the optimal conditions in achieving the maximum Fuel Gas heating value (FGHV).

The first part of this work presents a 1-D simulation model for a dry-fed EFG with oxygen and steam used as oxidizing agent. The model is then validated against published models for the similar reactor configuration and then extended to an existing EFG for an IGCC power plant in Pertullano, Spain. The second part then presents the optimization model in which the objective function is to maximize the FGHV. Solving both simulation and optimization model in gPROMS platform indicated that milder conditions are possible while improving the FGHV. A 12% increase in HV was realized with a decrease of about 500K in operating temperature. A 30 MPa increase in operating pressure only resulted in less than 2% increase in FGHV. Milder operating conditions, therefore, can decrease operating and capital investments, thereby improving the operating cycle of the power plant.

[884]

CO2 vs Biomass: Identification of Environmentally Beneficial Processes for Platform Chemicals from Renewable Carbon Sources

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A superstructure-based optimization is presented for the identification of environmentally beneficial process routes for platform chemicals (e.g. hydrogen, methane and methanol). Conventionally, platform chemicals are produced from fossil fuels such as crude oil and natural gas. In recent years, the production of chemicals from renewable feedstock has been considered. One option is the utilization of biomass as feedstock. Another option is carbon dioxide (CO2) as fossil fuel substitute. A rigorous comparison of processes employing renewable carbon sources is missing today.

The goal of this work is to identify the environmentally most beneficial process routes for platform chemicals. We consider conventional, biomass-based and CO2-based process routes. All processes are integrated in a single superstructure, which is analyzed using linear programming techniques. Optimization is carried out minimizing the considered environmental impacts (global warming and fossil resource depletion impact). This approach exploits synergies between the different process routes.

For renewable resources with limited availability, our analysis identifies the best use option. In particular, most CO2-based reactions require hydrogen as input. To produce hydrogen with low environmental impacts, we employ electrolysis using surplus electricity. Surplus electricity is a consequence of the increasing installation of intermittent, renewable energy sources. While the availability of CO2 is almost unlimited, the availability of biomass and surplus electricity is limited. Hence, the utilization of biomass and surplus electricity for the production of platform chemicals competes with alternative uses of these limited inputs. For example, biomass could be used to generate electricity and surplus electricity could be stored and reconverted to electricity. These alternative uses are therefore integrated in the superstructure.

The results show that the surplus electricity should be stored and not used for production of chemicals as long as electrical energy storage systems (e.g. pumped hydro storage or batteries) are available. However, biomass should be used to produce chemicals (hydrogen and methane) instead of conversion to electricity.

By accounting for the alternative utilization of limited resources, a holistic environmental assessment is achieved of process routes for platform chemicals based on renewable carbon sources.

[894]

Design and optimization of intensified quaternary Petlyuk configuration

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From its first introduction in 1965, the Petlyuk column received a high interest in the research community. Applied for the separation of three-component mixtures, the Petlyuk column is able to perform the separation with a reduced number of equipment and with a consistent reduction of the energy consumption compared to the classical sequences with simple columns. For a three-component separation the Petlyuk arrangement is composed by a prefractionator fully coupled with a main column that performs the separation of the products. Only one condenser and one reboiler are used in the scheme. When the prefractionator is combined in the main column's shell the resulting configuration is called divided wall column (DWC) and beyond the already cited possibility in energy reduction, it is possible also to reach considerable savings in the capital cost.

Considering the great potential of these sequences it is natural to think about a possible extension to more than three component separations. In the present work a four component case is examined. If the divided wall column configuration is considered, the presence of three walls inside the main column makes the design and the control too complex to attract the industrial interest for a real application. Even if some valuable work proved the applicability of multiple walls [1,2], the availability of more simple configurations is still a priority. Recently new intensified sequences are proposed for the separation of four-component mixtures [3]. These configurations use a less number of columns compared to the Petlyuk configuration. In the present work, further research on design and optimization of the obtained intensified Petlyuk configurations was focused. An aromatics plant is considered to prove that the new intensified sequences are able to substitute in a more operable way the complexity of multi wall configurations. Moreover the possibility to reduce the number of heat exchangers is also explored introducing one or more thermal couplings.

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[909]

Sequential mass integration for rigorous process modeling and flexible process design

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At local, regional and global levels, there is an increasing demand for chemical industry to provide products, services and innovations in a sustainable way by reducing the extensive use of material resources, waste production and energy utilities. At the same time, worldwide chemical industries must face challenging economic issues (competitiveness, costs and profitability) as well as strict regulations regarding reduction of their environmental impact. Therefore, they must frequently undergo retrofitting, often following the concept of minimum process changes with the maximum potential outcome in the process performance satisfying also process flexibility requirements. This can be achieved with various systematic approaches, among which heat and mass integration methodologies have been used over the last three decades in various forms (e.g., heat and mass integration independently, and combined, direct recycling and mass exchange networks, total site analysis etc.). A state-of-the art approach involves superstructure based methodologies often resulting in multi-objective mixed-integer (non)-linear problems for the design of the integration network requiring advanced optimization algorithms. Notwithstanding the merit of these powerful mathematical programming methodologies, sequential approaches still maintain some interesting properties, particularly with respect to interpretability, robustness and practicability. In this study, a sequential approach is defined as one comprising a sequence of well-defined actions (e.g., a matching of a process sink and a process source in mass integration terms) that satisfy the "conditional optimality" criterion, namely every new action should be optimal given the sequence of previous actions. The interpretability advantage of a sequential approach is already inherent in its definition. Additionally, robustness problems in the mathematical programming approaches usually arise when rigorous process models should be used because of their sensitivity to changed process inputs, a typical case in mass integration. Practical problems also arise when these rigorous process models are available in commercial process simulators, (e.g., Aspen Plus, ChemCad, etc.) which are not (optimally) designed to perform process optimization with the aforementioned superstructure methodologies.

In this work we exemplify how these issues can be dealt with sequential approaches for process integration. We focus on the direct recycling methodologies, which theoretically introduce less changes in the process modeling compared, for example, to the design of mass exchange networks. We present a sequential mass integration procedure targeting at an optimized series of source-sink matching, while safeguarding the potential of reaching an optimum integration target after an exhaustive sink-source matching. To this end, the study proposes a new metric and heuristics for ordering sinks and sources for the direct recycling problem when rigorous process models are used. The metric and heuristics are based on the affected process paths and a simultaneous monitoring of the impact of the adjusted process parameters along these paths on the multi-objective process performance criteria and the new integration problem resulting after every action in the sequence. The efficiency of this sequential method is demonstrated both in illustrative numerical examples and an industrial case study for optimal solvent recycling. The impact of diverse objective functions (i.e., other than targeting at maximum recycling) leading to the concept of "optimum partial integration" is also discussed.

[911]

Techno-economic analysis of power and hydrogen co-production by an IGCC plant with CO_2 capture based on membrane technology

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In recent years the interest for IGCC plants has increased, since it is a highly efficient and low emissions technology to produce energy from coal. This technology is also currently used to convert the pet-coke produced from petroleum processing in several refineries with limited emissions of pollutants. Moreover, the flexibility of IGCC plants allows using also renewable fuels like biomass materials to reduce the greenhouse gas (GHG) emissions. Alternative solutions to address the GHG reduction are based on the introduction of CO_2 capture units in the process before the gas turbine combustion [1]. In general, the results of these analyses indicate that the improved process requires significant additional capital costs for the new CO_2 capture units and, therefore, implies high marginal cost of electricity per ton of avoided CO_2 (i.e. mitigation cost). Also the co-production of electricity and hydrogen has been assessed in several studies with a range of technologies.

In this work the techno-economic analysis of an IGCC plant for power and hydrogen production with CO_2 capture by means of Pd-based H_2 membranes [2] was carried out. The case studies were referred to the modifications of the existing 330MWe Integrated Gasification Combined Cycle (IGCC) plant of ELCOGAS based on entrained flow gasification of a dry mixture of coal and pet-coke. The pre-combustion section consisting in a sour water gas shift reactor integrated with Pd-based H_2 selective membranes and CO_2 selective membranes [3] was simulated by process simulation techniques. Heat integration of the new process section was also addressed to minimize the energy loss. Power and energy penalty were evaluated as a function of the CO_2 capture percentage and of the electricity and hydrogen output.

Economic assessment of the additional capital and production costs was also performed to evaluate the mitigation cost of the carbon capture and storage (CCS) based on membrane technology. Sensitivity analysis was carried out to derive the breakeven price and the threshold performance of hydrogen membranes. The results on the cost of electricity, calculated without accounting for the revenues of the hydrogen sales, provided preliminary data for the economic feasibility of H_2 membranes in the IGCC process.

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[922]

Synthesis of Water Treatment Processes using Mixed Integer Programming

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With exerting pressures on water systems, efforts have recently been focused on optimisation of existing, and design of new treatment facilities. Modelling offers the advantage of early stage processes synthesis at minimum design change expenses. Current research and industry gaps lie in overall construction of water treatment flowsheets by crossing various disciplines.

In the present work a systematic approach for the synthesis of water treatment processes is proposed. The design combines technological robustness, improved economic performance and environmental reliability. The problem is formulated as a mixed integer non-linear programming (MINLP) model. A case study of seawater desalination is presented where conventional and non-conventional treatment technologies are considered. The flowsheet structure is selected based on units separation and recovery efficiency, operating and capital costs, carbon footprint and concentrate disposal regulations. The model is solved for desired water purity to meet drinking water standards with the objective to minimise water production costs. The results are analysed to investigate the applicability of the presented approach.

The developed methodology can have a significant impact on reducing the design time andsimultaneously, increasing the cost effectiveness of water treatment processes.

[923]

Viability of Technologies for CO2 Capture and Reuse in a FPSO: Technical, Economic and Environmental Analysis

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The recent discoveries of Pre-Salt layers in Brazil require process developments for enhanced sustainability as these reservoirs have oil with associated natural gas exhibiting an expressive amount of CO2. Monetization of CO2 by offshore production of methanol in a dedicated FPSO – MFPSO – is a potential alternative to sustainable E&P. Two process alternatives for anMPFSO were previously investigated by the authors, The alternative processes, consisted of physical absorption of CO2 with propylene carbonate and its conversion to yield methanol by Dry and Bi-Reforming, werecomparative on technical, economic and environmental grounds. Alternative 1 combines dry and steam reforming in one reactor (Bi-Reforming), while Alternative 2 segregates the two reactions - dry reforming occurs in one reactor and water gas-shift reaction takes place in a subsequent reactor.Additionally, both alternatives considered Enhanced Oil Recovery (EOR) as a parallel path for CO2 destination. The economic evaluation employed the software Capital Cost Estimation (CAPCOST) for calculations of CAPEX and OPEX. The software Waste Reduction Algorithm (WAR, EPA) was used to evaluate the potential environmental impacts - PEI (Potential Environmental Impact). The analysis indicated that the performance of Alternative 1 was superior to the performance of Alternative 2: (a) methanol production (17905 kg/h) 4 times higher, (b) lower CAPEX, (c) Sales Revenue 181% greater, and (d) the index for environment impact (868 PEI/h) 47,7% lower.In the present work, Alternative 1 was improved by removing the EOR step, with subsequent enhancement of methanol production as CO2 was integrally designatedto chemical conversion. The new proposed process (Alternative 3) inherits environmental feasibility of Alternative 1 and, through elimination of the EOR compression train,has the potential of positiveimpacts on CAPEX.

[1001]

A Superstructure-Based Framework for Simultaneous Process Synthesis, Heat Integration, and Utility Plant Design

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We propose a new framework for simultaneous chemical process synthesis, heat recovery network design, and utility plant design. We generate compact surrogate unit models to describe processes based on new technologies. We also consider (1) process streams with variable heat loads and temperatures, and (2) multiple steam types of variable temperature. We illustrate the applicability of our framework using a novel process for the non-enzymatic production of sugars from lignocellulosic biomass.

[1003]

Process design and optimization of integrated shale gas process for green chemicals production

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Over the past five years, the substantial development of shale gas has significantly increased potentially available supply, changed demand patterns, and multiplied the ways both traditional and alternative chemistries might be exploited [1]. Shale gas not only provides low-cost fuel, but also used as the raw material in chemical industry. Shale gas is somewhat unique and most of the shale formations in the U.S. are reported to be rich in natural gas liquids (NGLs, C2+ hydrocarbons) contents. These NGLs, sold separately, typically have substantially higher market values than the methane. Especially, the light NGLs such as ethane and propane are very important commodity chemical intermediates in the industrial value chain to produce polymers, plastics, synthetic rubber, adhesives, etc. The last concern with shale gas is about its greenhouse gas (GHG) emissions, as many researchers have concluded that the climate impact of shale gas maybe worse than those of coal and oil [2].

This work considers shale gas processing with on-site olefins production by co-cracking of NGLs-derived ethane and propane. To maximize olefins production, the oxidative coupling of methane (OCM) is also integrated to convert methane into short chain alkenes that includes ethylene and ethane. Traditionally, the major limitations of OCM process are its low olefins yield (below 20%) and selectivity (below 50%) with significant amount of unreacted gas (CH_4, CO, and H_2) and CO_2 byproducts, resulting in low project economics, and inevitably heavy carbon footprint. In the proposed process, these issues are addressed by co-processing strategy of OCM-products and co-cracking gas. The product separation cost is thereby significantly reduced and overall ethylene yielding rate is improved by recovering OCM-derived ethane and methane. The resulting process GHG emission is captured and compressed to supercritical pressure in order to be ready for sequestration. Besides, the life cycle GHG emissions of shale gas process can be further inherently mitigated by sustainable integration of renewable bioethanol as a hybrid feedstock. Overall, the proposed process consists of four Process Islands, namely gas treatment, gas to chemicals, methane to ethylene and bioethanol to ethylene. A simulation-optimization method based on the NSGA-II algorithm is developed for the process modelled in HYSYS. An energy integration model is also integrated using the mixed-integer linear programming. The results show that for a "good choice" design, the minimum ethylene selling price is $877.2/ton and the unit GWP of ethylene is 0.360 kg CO_2-eq/kg, when shale gas is considered as a high carbon fuel.

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[1008]

Life cycle optimization of integrated algal biorefinery processes for biofuel and biochemical production

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Over the past decades, biodiesel production processes via transesterification was developed and improved driven by the overwhelming environmental advantage of biodiesel over the fossil fuel counterpart, but the high production cost remained one of the most critical factors that hamper the industry from thriving. Among the promising biomass feedstocks, microalgae are an exceptional choice with high area productivity, minimum competition with conventional agriculture, low carbon dioxide emissions and valuable co-products. As a result of biodiesel prosperity, there is a need to convert the resulting glycerol to useful biochemical derivatives when the supply of refined glycerol easily exceeds the demand and the price decreases significantly [1]. Nevertheless, little attention has been paid to the integrated algal biorefinery for simultaneous biofuel and biochemical production in the open literature. Therefore, the objective of this work is to explore the optimal process design of integrated algal biorefinery processes under both economic and environmental criteria.

In this work, we propose a comprehensive superstructure of an integrated algal biorefinery by incorporating a biochemical production section into an algal biorefinery, which consists of cultivation, harvesting, lipid extraction, remnant treatment, biogas utilization, and biofuel production. The expanded biochemical section is capable of synthesizing four types of glycerol derivatives, namely, hydrogen, propylene glycol, glycerol-tert-butyl ether, and poly-3-hydroxybutyrate. Alternative technologies are also considered for harvesting, lipid extraction, biogas utilization, and biofuel production, resulting in 2,160 different designs in total. Based on the proposed superstructure, we develop a bi-criteria mixed-integer nonlinear programming (MINLP) model by following the life cycle optimization framework. A cradle-to-gate life cycle analysis is performed and integrated with conventional techno-economic evaluation model for process assessment to account for environmental impacts of greenhouse gas emissions associated with feedstock acquisition and transportation, as well as direct and indirect emissions from operating the integrated algal biorefinery. To efficiently obtain global optimal solutions, branch-and-refine algorithm and parametric algorithm are applied. The resulting Pareto-optimal curves demonstrate trade-offs between economic and environmental objectives and specifically provide the lowest unit annualized cost of $2.79/GGE, corresponding to a unit GWP of 0.146 kg CO_2-eq/MJ biodiesel.

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[1013]

The Effect of Charge Composition on the Optimal Operational Parameters of a Batch Extractive Distillation Process

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Batch distillation is used frequently for the separation of liquid mixtures in the pharmaceutical industry and waste solvent regeneration, among others. Azeotropic and close boiling mixtures are frequently encountered in these industries, but their separation requires a special distillation method, such as batch extractive distillation (BED), where an entrainer is fed continuously to the column, influencing favourably the relative volatilities.

The recovery of methanol by BED from a waste solvent mixture (acetone (A) – methanol (B) – THF (C) – water (D) – toluene (E)) of a pharmaceutical plant was studied. The components form several minimum azeotropes, of which the B-C and B-E azeotropes limit the recovery of B. At the end of the heating-up, B-C, which contains a high amount of B, appears at the top of the column. C and E are removed in the fore-cuts, and B is obtained in the main cut.

By BED, the addition of water decreases both the B-C and the B-E relative volatility. Water feeding is started already during the heating-up of the column, leading to a lower B concentration at the top already before the start of the fore-cuts, and thus to a decreased loss of methanol. This is an unusual application of BED, as the concentration of the main component is reduced in the column, instead of the impurities. Water feeding can be stopped at the end of heating-up (a new operation policy suggested by Lang et al. (2012)), or it can continue during the fore-cut. As water dilutes the mixture from which methanol is recovered, the duration and flow rate of water feeding has to be determined by optimization. For a typical charge composition, Hegely and Lang (2014) performed the optimization of the industrial process. However, the stopping criteria of the fore-cuts were not optimized.

In the present work, we investigated the effect of changing the composition of the charge on the results of the optimization. The optimization of the BED process was performed by a genetic algorithm. The algorithm was coded in Visual Basic under Microsoft Excel, and the program called a professional flowsheet simulator for the dynamic simulation. The objective function to be maximized was the profit. The optimization variables were the reflux ratios of the steps (fore-cuts, main cut, after-cut), the location, the flow rate and duration of entrainer feeding and the length of the fore-cuts (by varying the stopping criterion). The effect of changing the concentration of methanol and the two main organic impurities (C and E on the optimal values of the operational variables were studied. On the basis of the optimization, pilot plant productions were performed, whose results were compared with calculated ones.

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[1031]

VPPD Lab -The Chemical Product Simulator

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The objective of this paper is to present the systematic framework for chemical product design and evaluation, and its implementation in the software, the VPPD-Lab (the Virtual Product-Process Design Laboratory). The computer-aided techniques for the design of single molecular structure chemicals (lipids, solvents, aroma, etc.), formulations (paints, lotion, etc.), blended products (gasoline, lubricants, etc.), and emulsified products (hand wash, detergent, etc.) are implemented in the software. It employs a template approach that follows product-specific steps in the framework for data, target property models, and calculation routines. VPPD-Lab has options for product design, product evaluation and product validation. These last two options work in a similar fashion to a typical process simulator. That is, given the product details, it performs simulations of its properties to evaluate and validate its behaviour and performance. The application of the software is highlighted for a case study involving the tailor made design of jet-fuels.

[1063]

Synthesis of Flexible Heat Exchanger Networks Integrated with Reconfigurable Control Design

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In this work, a new systematic methodology, which integrates synthesis of a flexible heat exchanger network (HEN), with controllability aspects to achieve an efficient decentralized control structure is presented. The complete methodology is mainly based on the recent works presented by Braccia et. al (2014) and Luppi et. al.(2014). The first work is based on a previous model, named SynFlex (Escobar et. al ,2011, Escobar et. al ,2013), which uses a promising superstructure to obtain flexible HEN together with global optimization techniques (Björk et. al ,2002) to guarantee that Synflex model do not exclude optimal configuration. This strategy allows the optimal flexible HEN be able to operate well inside an expected range of operational conditions that could occur because of the environment of a plant. Then, this design is checked to be enough controllable based on the strategy developed by Luppi et. al. to determine a set of good candidate controllers. This is done in the context of reconfigurable fault-tolerant structures which is characterized by: (i) the generation of fully-decentralized designs to provide fault-tolerant capability based on the structural flexibility,(ii) the integration of the variables selection task (CVs and MVs) with the corresponding pairings definition (CVs-MVs), (iii) the consideration of scalar indexes to evaluate the potential solutions. These indexes are related to performance and stability criteria. An analysis based on necessary conditions is utilized to discard infeasible solutions. The complete procedure of this second part of the methodology is implemented through genetic algorithm framework. The advantage of the method is that it only utilizes steady-state process information. In addition, the structure configuration results independent from the particular design of the controllers. One example is given in this work to illustrate the potentiality of the proposed methodology and to support the final conclusions. In addition, as a future work is proposed to analyze the dynamic behavior of the controlled HEN integrated to the plant, since the overall works on this area use to present only the HEN.

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[1076]

Computer-Aided Approach for Designing Solvents Blend for Herbal Phytochemical Extraction

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There are many methods to obtain herbs phytochemicals such as the use of solvents as a phytochemical transfer medium in the extraction process. Currently, solvent is preliminarily selected based on the target phytochemicals and solvent polarities. This is followed by performing experiments to determine the potential solvents blends which give the highest desired phytochemicals extraction. The method uses a trial-and-error approach and is time consuming as well as resource intensive. The combination of property predictive models with computer-assisted search is one way to reduce the needs for huge amount of experiments needed to be conducted. Thus, the main objective of this work is to design solvent blends for the extraction of herbs phytochemicals using computer-aided approach. The methodology is divided into four levels which are pure component constraints (level 1), linear constraints (level 2), non-linear constraints (level 3) and stability checks (level 4). The proposed method has been applied to design a solvent mixture for the extraction of kaempferol from Kacip Fatimah herb as a case study. From the analysis, 12 feasible binary solvents mixture have been identified suitable for the extraction as it was within range of the design target. Thus, the optimal search has been performed to find the mixture solvents that can produce the highest kaempferol extraction yield with the lowest cost. Here, five binary solvents showed the highest kaempferol yield with the lowest solvent cost.

[1082]

Evolutionary Algorithm for De Novo Molecular Design Considering Multi-Dimensional Constraints

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The area of computer-aided molecular design has greatly influenced the rate and cost at which novel chemicals with desired attributes have been identified. As such, great effort has been invested in new methodologies which allow for the solution of larger and more complex problems of this nature. The application of evolutionary algorithms is one such technique which has shown promise in the solution of large combinatorial, and highly non-linear molecular design problems. The typical approach begins with a population of randomly generated individuals and the more fit members are stochastically selected to undergo computational analogues of natural recombination and mutation. This process is iterative until the resultant population possesses the desired attributes, which could be evaluated with existing quantitative structure property (activity) relationships (QSPRs) or other types of property models.

It has been shown that many molecular properties or attributes are often best characterized by a combination of descriptors with varying dimensionality. This could, for example, include a combination of graph theoretical two-dimensional descriptors, such as the chi connectivity index, along with three-dimensional descriptors, which capture important spatial characteristics. The inverse solution to property models of this nature, which entails identifying candidate molecular structures with the desired properties as defined by the given model, is often highly non-linear in nature. In addition, the use of molecular fragments, as often practiced in the de novo design of novel structures, can lead to a combinatorially large search space which becomes intractable for exhaustive solution techniques. The application of an evolutionary algorithm provides a powerful method for the solution of these types of molecular design problems in which there are often multiple objective constraints with high computational complexity and a large search space.

This approach utilizes a fragment based descriptor known as the Signature descriptor, which is represented as a molecular graph, as building blocks to generate candidate solutions. The nature of signature descriptors allows for control over the desired chemical search space as well as convenient reconstruction of the resultant molecular graphs. This descriptor has proven useful in the solution of problems with topological constraints and has recently been extended to tackle problems of higher dimensionality, including three dimensional as well as four dimensional (conformational ensemble) constraints. The graph-based operators necessary for such an approach will be outlined and the sensitivity of this approach with respect to various input parameters will be considered. Extension of previous studies to capture the effect certain parameters will have on the algorithm will provide insight into the often elusive decisions behind tuning evolutionary algorithms.

[1083]

Data Mining and Regression Algorithms for the Development of a QSPR Model Relating Solvent Structure and Ibuprofen Crystal Morphology

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In recent years, Computer Aided Molecular Design (CAMD) techniques have been used to inform and guide various experimental fields. Its use is increasing due to the fact that it reduces the time and cost of designing an ideal product for a given purpose. Currently, high quality models can be developed and implemented as a result of improved computing hardware, new methodologies, and availability of data. Decreasing dependency on experimental design also results in reducing the environmental footprint of companies involved in such research.

Though a well-practiced process, crystallization is a much less studied unit operation. It would be beneficial to consider the variables that affect quality and usefulness of the end product gained from crystallization. Some previous studies suggest that the interactions between solute and solvent are quite difficult to quantify and a large variance can be noticed with every solute-solvent combination. Pharmaceutical companies are widely known for using crystallization operations to develop their end product. Studying the crystal morphology is important as it has significant impact on the metabolizing processes in the human body.

This work focuses on developing a QSPR model to relate Ibuprofen crystal aspect ratio to the structure of the solvent utilized in the crystallization process [1]. The work utilizes a variety of data mining and regression algorithms such as PCA/PCR, GA-MLR, RBFNN, ANN to generate a proper QSPR model. In this contribution, the validation results of the models generated from these algorithms are thoroughly analyzed and explained. Three-dimensional descriptors are necessary to properly characterize the crystal morphology, however these descriptors have been shown to potentially lead to degeneracy issues. For this reason, the SVD method was used as an alternative to PCA for its increased stability in primary component prediction. Both internal and external validation methods were used to test the predictive capabilities of the developed models.

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[1084]

Designing Reactants and Products with Properties Dependent on Both Structures

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Computer aided molecular design can be performed in reactive systems to generate the structures of reactants and products yielding an optimal set of properties. In such designs the chemical reaction(s) are known and possible structures of the reactants and products are explored until their structure dependent properties are optimized. Dev et al. recently introduced an algorithm which is not restricted by the number of reactants and products that can be included in the design, a significant limitation of early works in this area [1]. They also enabled the inclusion of nonlinear property models and constraints. However, the algorithm was limited to the optimization of dominant properties of the products.

In this work, we introduce an algorithm that can generate structures of reactants and products irrespective of their numbers such that the dominant properties of each reactant and product is optimized. Property models, Both linear and nonlinear property models are used to relate the target properties to molecular structure. The effectiveness of molecular design techniques depends on the accuracy of the underlying property prediction models. A fuzzy optimization scheme has been utilized to account for the effect of property model accuracy by altering the target property bounds through consideration of effect of standard deviation.

As a result of the need to include a wide variety of property models on a single platform, molecular signature descriptors have been utilized in this work. Molecular signatures are fragment-based descriptors that can be used to reformulate various property models. They enable the simultaneous utilization of Quantitative Structure Activity/Property Relationships (QSARs/QSPRs) and Group Contribution Models (GCMs) [2]. In the formulated problem, all property/activity models are expressed in terms of the occurrence numbers of signature descriptors. Relationships have been developed that relate the occurrence number of the reactant and product signatures. This is achieved by tracking the atoms in the reactants that are exchanged to form the products, thus providing a structural relationship between the reactants and products. Therefore, any property constraints on reactants and products influence the selection of both and as such the problem is formulated as a multi objective fuzzy optimization problem. This problem is solved using techniques developed by Ng et al. [3] to obtain pareto optimal values of occurrence numbers of signatures of the reactants and products. This contribution will illustrate the developed methods and highlight their use through a case study.

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[1087]

Comparison of Energy Consumption in Heat Integrated Reactive Distillation Configurations for the Production Process of Formic Acid

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Five main different configurations including sub-configurations are investigated in this paper for the production process of formic acid, in order to compare and optimize the energy consumption. Those five main configurations are: 1) the conventional column configuration, which includes Huang's configuration and its optimized version; Huang's process configuration is optimized in this paper and used as base configuration which serves as reference model for other configurations; 2) thermally coupled configuration, 3) external heat-integrated (HI) configuration, 4) doubled effect configuration which includes the double effect conventional case, the double effect thermally couple case with one vapor side stream and/or two vapor side streams and 5) the double effect thermally coupled with external HI configuration. From the simulation results, it was observed that the external heat-integrated configuration and the double effect thermally coupled with external HI configuration showed the highest energy saving as compared to other configurations; however, although the double effect thermally coupled with external HI configuration showed the highest energy saving as compared to the external heat-integrated configuration, the latter was chosen as the simplest configuration with less energy consumption.

[1095]

Conceptual design of an internally heat-integrated reactive distillation column based on thermodynamic and hydraulic analysis

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This work introduces an efficient approach to the conceptual design of an internally heat-integrated reactive distillation column (i-HIRDiC) synthesizing ethylene glycol (EG) through the hydration of ethylene oxide (EO). Unlike the conventional EG reactive distillation column which has only one column shell with two sections, the i-HIRDiC configuration comprises two columns. The reactive column is operated at a higher pressure (benefiting the reaction) while the stripping column is operated at a lower pressure (benefiting the separation), which results in the temperature differences between the two columns. The two columns are built in a typical concentric configuration with heat transfer panels placed on the plates of the stripping column. The hot vapor enters the panel and vaporizes the liquids flowing across the outer surface of the panel, enhancing the energy performance of the system. A systematic method is proposed to obtain a feasible physical configuration with maximum possible extent of heat integration, in which the column diameter, the number of panels and the panel size on each plate are iteratively examined and determined according to thermodynamic and hydraulic analysis. Simulation results proved that an ideal i-HIRDiC configuration (without the reboiler through the maximum internal heat integration) was infeasible due to limited heat transfer area in the column. A partial i-HIRDiC configuration with the existence of a condenser and a reboiler was feasible. Evaluated by the total annualized capital cost (TAC), the comparison results showed that neither of the two commonly used heat distribution schemes, i.e. uniform heat transfer area and uniform heat duty distribution, was as good as the design acquired from the proposed methodology.

[1117]

Carbon Capture and Utilisation: Application of Life Cycle Thinking to Process Design

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An increasing interest in carbon capture and utilisation has opened the door for exploring opportunities for using waste CO2 as a feedstock for the production of high-value products such as fuels. The production of synthetic fuels from fossil resources, such as coal or natural gas, is a well-established practice, especially in countries with limited reserves of crude oil. However, while the possibility of converting waste CO2 into synthetic fuels is attractive, the life cycle environmental implications of such fuels are uncertain, mainly because of the high thermodynamic stability of CO2 and the demanding process conditions, i.e. high temperature and pressure. Thus, there is a risk of producing synthetic fuels from captured CO2 with the overall CO2 emissions higher than if the waste CO2 was discharged directly into the environment. To explore this issue, the paper considers production of synthetic diesel in a Fischer-Tropsch (FT) process using waste CO2 from anaerobic digestion of sludge from wastewater treatment. Using an Aspen model, the study shows how systems life cycle approach can be integrated into process design and how environmental 'hot spots' can be translated into key design targets to improve the environmental sustainability of the system from 'cradle to grave'. Several process alternatives are considered, including different sources of hydrogen and recycling rates of monoethanolamine (MEA). The results indicate that the MEA is the main hot spot and, with no recycling (regeneration), total global warming potential (GWP) of the FT diesel is nine times higher than for conventional (fossil) diesel. However, by setting design targets for MEA recycling, it is possible to produce FT diesel from CO2 with the GWP comparable to that of conventional diesel. In the case of hydrogen sourced from natural gas reforming, the target of a minimum of 95% recycled MEA must be achieved; if using hydrogen from naphtha cracking or from water electrolysis, this target is 92% because the hydrogen from these sources has lower life cycle impacts. Increasing MEA recycling beyond the target levels will lead to lower impacts from synthetic than fossil diesel. These findings illustrate how consideration of life cycle environmental impacts in early stages can enable engineers to optimise design by focusing on life cycle stages that have highest impacts, thus leading to more sustainable systems by design.

[1152]

Model-Based Selective CO2 Capture from Biogas Streams Using Ionic Liquids

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Monoethanolamine (MEA) has been used for decades as a solvent for CO2 capture. Typically, for MEA the absorption process is done by chemisorption at 50°C followed by temperature swing desorption at 120°C, hence the energy penalty is high. In addition, the high volatility of MEA, its corrosive behaviour and its thermal degradation over time have been suggested as hindrances to the economic success of CCS and CDU. In contrast, ionic liquids (salts which are liquid at room temperature) have been shown to have high CO2 affinities and are noted for their negligible volatility, reasonable thermal stability, strong dissolubility and their ability to be custom designed to provide chemical environments which favour particular applications.

Current CO2 capture systems in anaerobic digestion plants typically employ water scrubbing or amine based solvents, such as MEA, to remove CO2 from the biogas and upgrade it to natural gas standards. This modelling work considers five different ionic liquids, both cation based and anion based, to act as physical solvents for CO2 capture from biogas. The COSMO-SAC activity coefficient property method is employed in Aspen Plus to perform mass and energy balance calculations over the whole process. The parameters needed by the COSMO-SAC property method, such as critical properties of the ionic liquids, volume parameters and sigma profiles are calculated using different correlations and the COSMOtherm® software. A conceptual process flowsheet for CO2 capture is then built in Aspen Plus for each ionic liquid consisting of an adiabatic absorber which was modelled using the RadFrac subroutine, a flash drum for solvent regeneration with pressure swing and a centrifugal pump for solvent re-circulation. In addition to mass and energy balances, the height and diameter of the absorber as well as the electrical consumption of the pump are also calculated. The results from the simulations are compared in order to identify the most promising ionic liquid in terms of absorption capacity, energy consumption and solvent loss.

Track 5. Process Dynamics, Control and Monitoring

[12]

Nonparametric soft sensor evaluation for industrial distillation plant

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The paper deals with the improving of existing methods of nonlinear soft sensors development via nonparametric approach based on the example of industrial distillation unit. The sequence from two industrial distillation columns of FCC unit is considered. In practical situation, the main difficulties of evaluation of soft sensor model are:

a) inherent process nonlinearity;

b) unknown model structure;

c) narrow variability ranges of some key inputs variables.

In order to overcome abovementioned obstacles a)-c) the using of nonparametric regression based on ACE-algorithm is proposed in the paper. The industrial case study of isopentane prediction in the distillation unit product is considered it detail with data-based identifiability analysis of soft sensor model. The advantage of application of proposed procedure for handling of narrow variability range of input variable as column pressure (test sample) was shown. The procedure is based on the nonparametric regression with combination of calibrated rigorous model analysis of distillation unit.

[25]

Comparing Temperature Difference Control Schemes for Dividing-Wall Distillation Columns

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The operation of a DWDC, fractionating an ideal ternary mixture of hypothetical components A, B, and C, is studied to compare various temperature difference control schemes proposed so far, including temperature difference control (TDC) scheme, simplified temperature difference control (STDC) scheme, double temperature difference control (DTDC) scheme and simplified double temperature difference control (SDTDC) scheme. The nearly similar system performance of the STDC and SDTDC schemes to the TDC and DTDC schemes, respectively, indicates the great importance to control strictly the two sections along the dividing wall. With the two intermediate sections tightly controlled, the operation of the rectifying and stripping sections should then be tightened to improve further system performance. This gives rise to a novel SDTDC scheme involving two DTDC and two TDC loops, which enriches the potential alternatives to control the DWDC.

[46]

A Decentralised Multi-parametric Model Predictive Control Study for a Domestic Heat and Power Cogeneration System

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Combined Heat and Power (CHP) systems have been receiving a lot of interest as a substitute of traditional power and heat generation resources in residential applications [1]. Their decentralized production characteristics, cost effective nature and small environmental footprint have added towards that direction. In a natural gas powered, internal combustion engine CHP for residential use two main subsystems can be identified: (i) the electrical power production subsystem and (ii) the heat recovery subsystem. The former generates the electrical power through combustion of natural gas in a reciprocating internal combustion engine while the latter produces hot utility water using the by-product heat resulting from combustion. The high fidelity model of the two subsystems and their interactions provide the basis for advanced control studies [2]. The operational objectives of such a system in domestic application are to meet (i) the electrical power demand and (ii) hot water demand. To tackle the complexity of the high fidelity model, the multiple objectives and the dual nature of the system, we propose a decentralized multi-parametric Model Predictive Control approach to the problem of the operation of a CHP system in the domestic sector.

The CHP system has been treated as the interaction of the electrical power production subsystem with the heat recovery subsystem, rather than as a monolithic system, following the framework presented in [3]. The operation of the CHP system is governed by either the demand of electrical power (Case 1) or the demand of hot water (Case 2). In Case 1, the system attempts to (i) cover the electrical power demand and (ii) produce water of a predefined temperature, regardless of the flow rate. In order for this to happen, the controller of the heat recovery subsystem controls the temperature of the water at the outlet of the heat recovery system via the manipulation of the water flow rate while treating the operational level of the energy generation subsystem as a measured uncertainty. In Case 2, the system attempts to produce water at predefined temperature and flow values. This is translated into treating both the water temperature and flow rate as control variables while the flow rate set point and the operational level of the electrical power generation subsystem are treated as manipulated variables. The latter is treated as a power output set point for the energy generation subsystem. The modeling and control schemes are performed in gPROMS® (www.psenterprise.com/gproms) and MATLAB® using the principles described in PAROC (www.paroc-platform.co.uk). The multi-parametric controllers, in both Cases, manage to sufficiently capture the dynamics of the system and cover the demand efficiently and accurately.

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[64]

A control strategy for periodic systems - application to the twin-column MCSGP

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In this work we present advanced multi-parametric control strategies for the "Multicolumn Countercurrent Solvent Gradient Purification" (MCSGP) process, which is a continuous chromatographic separation process, governed by a periodic operation profile, linked to the intensification of monoclonal antibody production. We demonstrate a seamless, step-by-step procedure for the development of multi-parametric controllers as part of our recently introduced PAROC framework and software platform. The designed controller assures optimal operating conditions, avoiding pertubations, under continuous operation, while capturing the periodic nature of the process.

[78]

Design of multiparametric NCO-tracking controllers for linear dynamic systems

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A methodology for combining multiparametric programming and NCO tracking is presented in the case of linear dynamic systems. The resulting parametric controller contains information regarding the solution structure provided by multiparametric programming and the corresponding feedback control laws for tracking optimality conditions, thus avoiding the need for repetitively solving optimization problems in online real time control. An example of a constrained linear quadratic optimal control problem with initial conditions as parameters is presented to illustrate the approach.

[91]

A Performance-Oriented Robust Framework for the Online Model-Based Optimization and Control of (Fed-)Batch Systems

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The development of an efficient methodology to deal with model uncertainty in optimal control and/or dynamic optimization algorithms still remains a serious challenge. In the last decade, several authors have tried to address this problem but most of them have only focused on finding strategies to avoid the controlled system to operate outside its lower and upper bounds at all costs. The worst case approach (Logist et al., 2011) and the sigma points method (Recker et al., 2012) are two wide-spread examples of such strategies. Although these kind of strategies have proven to be very robust, they also take to a significant reduction in the controlled system performance, thus being suitable only for processes where a bound violation implies unacceptable consequences. This work is aimed at describing a novel robustification methodology that is suitable for systems where the upper and lower bounds are soft constraints, i.e. the only relevant consequence of their violation is the loss of the current batch. The idea is to use a multi-scenario description for the process model where each scenario relates to a certain set of the uncertain parameters and is associated to a certain probability to occur. All the scenarios are simulated in real-time and the controlled system profitability is evaluated with a user-defined performance indicator, in each scenario. All the single scenario performances are combined by means of a weighted sum into a global performance index, which is employed as the objective function of the simultaneous optimal control and optimization algorithm. The weighting coefficients of the global performance index can be chosen as the normalized probabilities of occurrence for each scenario. The proposed approach, unlike the worst case and sigma points methodologies, measures the effect of the uncertainty directly on the system performance, thus it conveys information on how to take a risk and when and is expected to provide better performances on an average basis.

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[92]

A Reliable Modifier-Adaptation Strategy for Real-Time Optimization

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In model-based real-time optimization, plant-model mismatch can be handled by applying gradient- and bias-corrections to the cost and constraint functions in an iterative optimization procedure. One of the major challenges in practice is the estimation of the plant gradients from noisy measurement data, in particular for several optimization variables. Most finite-difference based approaches suffer from the problem of choosing the right step-size, in which using a large step-size may decrease the effect of noisy data on the one hand, on the other hand it leads to considerable truncation errors. In this paper we propose a novel real-time optimization scheme that explores the inherent smoothness of plant mapping to enable a reliable optimization even if the data is subject to a high noise level. The idea here is to combine the quadratic approximation approach used in derivative-free optimization techniques with the iterative gradient-modification optimization scheme. First, the available measurements at past operating points are screened according to the Λ-poisedness, age and distance related to the current set-point to determine a suitable set of points for quadratic approximation. This step is critical for making a proper use of the measurement in the quadratic approximation approach to extract approximate gradients. The trust region for the next move is determined by a covariance analysis of the distribution of the set. Using the set of data, quadratic approximations of the plant cost and constraint mappings are constructed by regression. Afterwards, the plant gradients are extracted from the quadratic approximations and applied to the modifier-adaptation optimization. The global convergence of the scheme is analysed. Simulation studies with the optimization of the Otto-Williams Reactor show its promising performance.

[100]

Raman-based Advanced Control of an Absorption Desorption System

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For absorption processes with fluctuating feed gas compositions it is vital to continuously adjust the operation point to achieve energy efficiency. In this contribution a Raman-based advanced process control (APC) is introduced for the absorption of carbon dioxide (CO2) using an aqueous solution of monoethanolamine (MEA). The APC is based on a Raman spectroscopic analysis of the composition and CO2 load of the scrubbing liquid and a non-linear model predictive control (NMPC) to adjust the scrubbing liquid cycle. In addition, an outer real-time optimization loop is set in place to update the set points for the absorption process depending on the current feed gas composition minimizing the energy consumption of the process. Implementation and testing of the APC have been carried out in a mini-plant at TU Berlin. During a plant operation of more than 160 hours robustness and stability of the APC were shown.

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Dynamic analysis of extractive distillation systems aided by ionic liquids

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In the last decade, ethanol dehydration has received a renewed attention because of the sudden increase of bioethanol production as alternative source of energy. Nowadays, an extensive number of papers dealing with the steady state and dynamic properties of this extractive distillation system has been reported. In addition, given that success of this process strongly depends on the selection of a suitable entrainer, the effect of solvent choice on its operational cost and control properties has also been studied. In recent years, several authors have reported that some Ionic Liquids (IL's) may be used as solvents for recovering anhydrous ethanol. However, although IL's implementation could be a feasible technology, there is still a lack of information about their effect on the system's controllability. The objective of this work is to explore the dynamic implications of implementing these new solvents in the ethanol dehydration process. The selection of control configurations for an extractive distillation column using 1-methylimidazolium chloride ([mim]Cl) as entrainer is presented. The Relative Gain Arrangement methodology was used to determine the appropriate control structures, and the dynamic performance of each feasible structure was evaluated through the response of the system under changes on the feed composition. The results show that solvent concentration, which is directly related to the attainable degree of separation, has an important effect on the control structure definition, as well as on the dynamic performance of the system.

[121]

Selection of Comprehensive Data from a Large Amount of Data using a Genetic Algorithm

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Soft sensors [1] are widely used to predict process variables that are difficult to measure online. An inferential model is constructed between the variables that are easy to measure online and those that are not, and an objective variable, y, is then predicted using that model. Through the use of soft sensors, the values of y can be predicted with a high degree of accuracy.

One of the crucial difficulties of soft sensors is that predictive accuracy drops due to changes in state of chemical plants. This is called as the degradation of soft sensor models [2]. To reduce the degradation, the model is reconstructed with newest data. A moving window (MW) model is constructed with data that are measured most recently and a just-in-time (JIT) model is constructed with data that are more similar to prediction data than other data. The models such as MW and JIT models that have adaptive mechanisms are called adaptive models [3].

To construct adaptive models with high predictive accuracy for wide data range, monitoring database is a crucial problem. Kaneko et al. proposed the database monitoring index (DMI) to monitor databases and the method that manages databases for adaptive soft sensors with the DMI [4]. Decision whether new measured data are stored in the database or not is made, based on the DMI-values of the new data, and accordingly the predictive accuracy of the soft sensor models increases. However, there is no way to costruct the first database to start prediction from a large amount of data that were measured in a plant and are data rich, but information poor.

Therefore we proposed a method to select comprehensive data from a large amount of data for adaptive soft sensor models with high prediction accuracy. A genetic algorithm [5] is applied to the data selection. As an objective function of a genetic algorithm, distance between data, distribution of data and predictive accuracy of a soft sensor are discussed to represent the amount of information in databases. Through the analysis of simulation data and real industrial data, we confirmed that the first databases could be appropriately constructed from a large amount of data and the preidctive accuracy of adaptive soft sensors increased by using the proposed method.

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[135]

A Comparative study between Neural Networks (NN)-based and Adaptive-PID Controllers for the Optimal Bio-Hydrogen Gas Production in Microbial Electrolysis Cell Reactor

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A comparative control system of Microbial electrolysis cells (MEC) for wastewater treatment has been analyzed in this study. MEC process uses the fundamental of a bio-electrochemical process and it is a promising renewable energy technology that can produce a hydrogen gas as a by-product while the wastewater is being treated simultaneously. The main challenge of the hydrogen production study for the MEC reactor is to obtain a good automatic control system due to nonlinearity and complexity of the microbial interactions. Thus, the MEC reactor are difficult to be operated and controlled especially under the optimal conditions. To address this issue an integrated approach involving process modeling, optimization and advanced control has to be implemented. This comparative study focus on the controller's performance in the control system; neural network (NN)-based and Adaptive-PID controllers. The study has been carried out under optimal condition for the production of bio-hydrogen gas wherein the controller output are based on the correlation of the optimal current and voltage to the MEC. Various simulation tests involving servo and regulatory cases have been evaluated and the performances of both controllers are discussed. A Ziegler–Nichols tuning method and an adaptive gain technique have been used to design the PID controller, while the neural network controller has been designed from the inverse response of the forward MEC model. The neural network-based controller results in fast response time and less overshoots while the offset effects are minimal. In conclusion, the neural network (NN)-based controllers provides a better control performance on the MEC system compared to the Adaptive-PID controller.

[141]

Reaction Monitoring of Cementing Materials through Multivariate Techniques Applied to In Situ Synchrotron X-Ray Diffraction Data

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In recent years, the interest in reaction monitoring achieved by means of spectroscopy combined with multivariate statistical techniques has significantly grown, since they allow to monitor the reaction progress, detect abnormal conditions and verify whether reaction achieve the equilibrium state.

This work is focused in monitoring the formation and growth of crystals in magnesium potassium phosphate cement, MKPC, which is believed as one of most promising cementing material. MKPC is obtained from MgO-KH2PO4-H2O ternary system, its nucleation and growth process modeling is not trivial since it is controlled by a combination of thermodynamic and mass transfer properties. Nevertheless, spectroscopic techniques with multivariate statistical techniques permit a fast, real time and reliable analysis of the phenomena occurring in the system. It can be employed even when reactions between species are difficult to identify or little is known about them.

The experiment was performed at room conditions (T=20°C) and using a unity molar ratio of magnesium to phosphate. Time-resolved X-ray powder spectroscopy was used to assess crystal structure during the reaction since it is a nondestructive technique, suitable for in situ measurements. Each spectrum was recorded covering a 2θ range 0.97°-43.82° and XRPD profiles were collected between time t=0-111.23 min.

Hence, Multivariate Eigen-Factor Analysis (MVA) was used to collect the useful information. In particular, some pre-processing and variable selection strategies of the spectral data were evaluated. The results show that the system dynamics seems to be qualitatively described by the time evolution of the latent variables, making possible the identification of different reaction stages from XRPD profiles such as reactants consumption, transition through amorphous phase and finally MKPC formation.

In this work, MVA has been revealed as a useful tool for interpreting spectral data from reactions, it clearly encourages further investigation about system dynamics and application of others related multivariate statistical techniques.

[145]

Multivariate fault isolation using lasso-based penalized discriminant analysis

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In industrial processes, multivariate statistical process monitoring is becoming increasingly important for ensuring the safe and efficient operation of manufacturing and chemical industries, where isolating faulty variables is a critical step to discover the source of the detected fault. Although fault detection methods have been intensively investigated, studies on fault isolation are relatively limited, due to the difficulty in analyzing the influences of multiple variables on monitoring statistics. The most popular technique for fault isolation is contribution plots. Although easy to use, contribution plots often suffer from "smearing" effect and yield misleading results. Reconstruction analysis is another type of isolation method, which re-calculates the values of process variables and monitoring statistics along certain candidate "faulty directions". Such method requires the candidate "faulty directions" to be known, which may not be satisfied in industrial applications. A branch and bound (BAB) algorithm was proposed to address the fault isolation problem by solving a combinatorial optimization problem. However, the computational burden of BAB is heavy. In addition, reconstruction analysis may lead to inaccurate results when the number of variables is large, as shown in this paper.

To solve the mentioned problems of the existing methods, this paper proposes to conduct fault isolation via penalized discriminant analysis. The basic idea is as follows. The goal of fault isolation is to identify variables responsible for the detected process abnormality. In other words, the variables to be isolated are those discriminating the normal process measurements and the fault samples. In a sense, isolating faulty variables is equivalent to identifying discriminating variables in a two-class problem, with the normal operation data regarded as belonging to one class and the data corresponding to the detected fault as belonging to the other class. In this paper, such idea is illustrated using the famous Fisher's Discriminant analysis (FDA) technique. It is worth noting that, different from supervised fault classification in many existing studies, here FDA is utilized for unsupervised fault isolation. As proven in previous research, an FDA model can be transformed identically to a least squares regression model with predictors and response variable selected properly. Consequently, the task of identifying discriminating variables can be accomplished by doing variable selection for a regression model, which can be expressed in a form of the least absolute shrinkage and selection operator (lasso). As a penalized regression method, the lasso minimizes the residual sum of squares under a constraint on the L1-norm of the coefficient vector, which tends to produce some zero coefficients enforcing sparsity in the solution. By doing so, it conducts parameter estimation and variable selection simultaneously. Since the lasso can be solved efficiently using state-of-the-art algorithms, the problem of computational burden is avoided. Instead of just offering a suggested set of faulty variables, the lasso provides more information on the relevance of process variables to the detected fault, which facilitates the subsequent root cause diagnosis step after isolation.

The benchmark Tennessee Eastman (TE) process is used as a case study to illustrate the effectiveness of the proposed method. The results show that, comparing to the existing methods, the lasso-based penalized discriminant analysis method is more information-rich and easier to calculate.

[163]

Flexible operation of CO2 capture processes integrated with power plant using advanced control techniques

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Control and limiting of carbon dioxide emissions in energy production and other energy-intensive sectors are major challenges of science today. Several different methods to avoid, separate and store CO2 from the flue gases of energy production have been proposed in the literature. Post-combustion CO2 capture from fossil fuel power plants using amine-base solvents, typically monoethanolamine (MEA), is one of the most promising technologies for the CO2 removal. In this work, a consistent dynamic rate-base model is used to describe CO2 capture process in aqueous solution of MEA. The present model has been implemented in the Matlab/Simulink in order to do a part-load analysis and elaboration of control strategies of carbon capture process to be used within a power plant. The model is estended from already developed models with the group. The experimental results published in literature for Esbjerg CESAR pilot plat (pilot plant parameters: absorbent 30wt% MEA; packing type: Sulzer Mellapak 2X; absorber diameter 1.1 m, packed height 17 m) are used to validate the developed model. A good correlation between absorber's temperature profiles obtained by simulation and experimental was observed, R value is 0.936 in case of liquid's temperature and 0.965 for gas's temperature. Flexible operation of post-combustion capture is one approach which has been proposed as a means of addressing the energy penalty during peak periods for electricity demand. A complete uderstanding of the dynamic operability of power plant with CO2 capture using amine-based solvents is fundamental to successfully implement this process in commercial scale power plants. The proposed dynamic model was used to simulate the transient behavior of the CO2 capture plant due to changes in the flue gas flow rate, in order to study the effect of power plants operating conditions on the CO2 capture process. The CO2 removal capacity has been studied using a ramp, step and sinusoidal input tests to highlight the transient response. The dynamic behavior study of the CO2 capture process reflect that plant performance are reduced significantly with excessive increase of the absorber load and a decreasing of Fg/Fl allowed an increasing of CO2 capture rate. The sinusoidal test was introduced in the process model to study the oscillatory behavior of this process, which is a typical behavior for power plant outputs. Thus, this case study was carried out considering that the amplitude of the sinusoidal function is 15% with respect to the flue gas input base case value and that the sinusoidal input was set to complete one cycle within a day. The simulation was performed for five days. The percentage of CO2 removal reached a minimum value (82%) when the flue gas flow rate was at its maximum rate and a maximum value of 95.5% at the minimum flue gas flow rate. From environmental protection point of view the primary control objective for the absorption column is control of the carbon dioxide quantity in the sweet gas stream. In this study, typical disturbances have been investigated, such as the step increment of 10% in the flue gase flow rate with respect to its nominal operating point. The amount of liquid flow was adjusted to provide absorption of at least 90% CO2 of the gaseous mixture. The performance of a model predictive control (MPC) strategy was compared with the classical PID control strategy. The study results revealed that the MPC controller was capable to maintain the variation of the controlled variables much closer to the set points than the traditional PID. The preview capability of MPC, its optimal characteristic and ability to handle constraints are revealed when used for set point tracking and disturbance rejection aimed to ensure efficient operation.

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Modified Minimum Variance Approach for State and Unknown Input Estimation

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For several systems of interest, inputs to the system may be unknown. Thus, one may be interested in estimating the unknown inputs alongwith the states. In this work, we modify the approach proposed by Madapusi and Bernstein (2007) for estimating the states and the unknown inputs. The approach, applicable to systems with feedthrough, obtains a minimum variance unbiased estimate of the states. The inputs are estimated after the filtered states are obtained and do not require any restrictive assumptions about the dynamic variation of the inputs. Compared to Madapusi and Bernstein (2007), our approach differs in the prediction step. In particular, we use the estimated input in the prediction step while it has not been considered in the work of Madapusi and Bernstein (2007). Our proposed modification reduces the number of constraints that need to be satisfied by the filter gain thereby increasing the applicability of the approach. The efficacy of the approach is demonstrated by applying it to estimate unknown inputs and states in a self powered neutron detector, that is widely used in nuclear reactors to monitor the neutron flux.

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[211]

A New Software Development Methodology for Controllability Analysis of Forced Circulation Evaporator System

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Modern processing plants are becoming more and more complex due to the tighter economical and environmental limitations. As a result, unit operations become more coupled and more non-linear. The more dependent and non-linear the unit operations, the harder it is to maintain the process outputs within the feasible and optimal operating regime. The ability to handle the process system outputs by using feedback control is called controllability of process design. Studies show that poor controllability of a plant can result in long-term economicdrawbacks and safety hazards.

There are many controllability assessment methods available in the literature. These methods are divided into two main groups: linear and non-linear measurements. Dynamic resilience, as a linear measurement, is defined as the quality of the regulatory and servo behaviour which can be obtained by feedback control (Garcia and Morari, 1982). On the other hand, controllability of a process is inherited directly from the design itself (Yuan et. al, 2010), which means that regardless of the controller and controlling strategy, the controllability index is constant. Therefore, evaluation process of the plant-wide design, from controllability point of view should be takenintoconsideration at the design stage.

Despite the need for software tools for controllability assessment at the earlier stage of process design, there is no world class software tool available in this field. Our studies suggested that is it due to two major reasons: firstly, it is because of the problem-specific nature of the controllability problems. Almost in every case, a unique method ofmeasurement is used for controllabilityassessment. This means that for every controllability problem there should be a unique software developed, which makes it economically unbeneficial for the software companies to enter this domain; and secondly, because of the interdisciplinarycharacteristics of the controllability problems, a group of expertise from different fields, such as chemical, control and software engineering, with acceptable level of knowledge of the problem should be assembled, which makes the process of software development even harder and more expensive.

In this work a graphical domain-specific language (DSL) is introduced for measuring RGA index, to assess the controllability of a process system. DSL is a computer programming language of limited expressiveness focused on a particular domain (Fowler, 2012). In other words, DSL brings new technologies of developing programming languages together, so the development cost drops dramatically. This programming language uses symbols and notations, which are well known by the domain experts, i.e. process engineers. Therefore, it addresses the communication problem between programmers and process engineers. In this work, DSL is applied to a non-linear evaporator system.The process consists of an evaporator, separator, condenser and a recycling pump. The goal in this system is to control the concentration of the outlet stream, the evaporator pressureand the liquid level in the separator by manipulating the pressure of theinlet steam, the coolant flow-rate and the outlet flow-rate.

The proposed programming language is shown to be capable of analysing the process system design and reporting the RGA index. Also, the controlled uncertainties are applied on the input variables and their impact on the controllability index is discussed.Finally the advantages of using the proposed DSL methodology over the conventional models are presented.

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

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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 environmental sustainable.

In this work, a systematic model-based methodology for integrated design and operation of reactive distillation operations is presented. Issues related to operation are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions. The methodology employs a decomposition-based method so that the complexity of the problem is reduced into a set of sub-problems that are solved sequentially. The method consists of four hierarchical stages: (1) pre-analysis, (2) steady state analysis, (3) dynamic analysis, and (4) evaluation stage. To illustrate the application of the proposed methodology, production of methyl-tert-butyl-ether (MTBE) using a reactive distillation column (RDC) is considered. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used. The methods are based on the element concept, which is used to translate a ternary system of compounds (methanol, isobutene and MTBE) to a binary system of elements (elements A and B). For a binary element system, a simple reactive McCabe-Thiele-type method (to determine the number of reactive stages) has been used. The reactive equilibrium curve is constructed through sequential calculation of reactive bubble points. For an energy-efficient design, the driving-force approach (to determine the optimal feed location) for a reactive system has been employed. For both the reactive McCabe-Thiele and driving force method, vapor-liquid equilibrium data are based on elements. The reactive bubble point algorithm is used to compute the reactive vapor-liquid equilibrium data set.

The operation of the RDC at the highest driving force and other candidate points is compared through open-loop and closed-loop analysis. By application of this methodology it is shown that designing the process at the maximum driving force results in an energy efficient and operable design. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.

[216]

A nonlinear quasi-unknown input observer for the chemostat Droop model

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The problem of state and input estimation for the Droop model of microalgae growth in the chmostat with biomass cocnentration measurement is addressed. The feed nutrient concentration is considered as piecewise constant and unknown, and is thus considered within the framework of quasi-unknown input observation.

It is shown that the system is unknown input observable for this configuration, and an extended order quasi unknown-input estimator is designed for the reconstruction of the state (biomass, nutrient quota, and extracellular nutrient) as well as the unknown input. The resulting nonlinear observer has a PI-like structure, and its semi-global convergence is assessed through a Lyapunov function approach leading to a LMI which is feasible for adequately chosen observer gains.

Numerical simulation studies are presented which corroborate the theoretic assessment, and show the performance capabilities of the proposed observation scheme.

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PAT for reactive crystallization process optimization for phosphorus recovery from sewage sludge

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Recycling phosphorus from wastes and transform it into reusable product is a global challenging as the mineable P deposits are predicted to be depleted within 60-130 years. Recovery of phosphorus from sewage sludge ash could offer an opportunity of developing a sustainable phosphorus supply. Reactive crystallization is an emerging technique for P recovery, however, the development and optimization of such reactive crystallization processes is extremely challenging due to the complex composition of the sludge. The sludge ash may contain high concentration of iron and aluminium since iron or aluminum salts are frequently used to precipitate phosphate at wastewater treatment plants (WWTPs). In the present work, we proposed a reactive crystallization process for recovering phosphorus as CaClH2PO4×H2O at a very low pH. The process consists of two steps, in the first step the sewage sludge ash was pretreated with hydrochloride acid to extract the phosphorus into the liquid solution, and subsequently the reactive crystallization was performed by feeding calcium chloride solution. The concentration of phosphorus and the different cations has been characterized and has been used to build up the solution equilibrium models based on the thermodynamic equilibrium constant of the species in solution and the solubility product of the substances that might precipitate out from the solution. The mechanism of the reactive crystallization process was investigated using process analytical technologies (PAT), such as in line Attenuated total reflection Fourier Transform Infrared (ATR FTIR) spectroscopy and Raman spectroscopy combined with multivariate chemometric algorithm. The concentration profile of the different ions that are essential for the reactive crystallization process was monitored with the in-line PAT tools and has been used to establish the kinetic modeling of the crystallization process. The effects of different operation parameters, such as pH, concentration of the reactants, temperature, seeding with the product crystals, have been investigated, and a design space has been established. Based on the in-depth understanding of the process, the optimization of the reactive crystallization process has been performed in terms of the purity of the products, phosphorus recovery of the process, and the operating costs. The results obtained in the present work showed that the purity of the phosphorus product can be optimized and the precipitation of iron and aluminium phosphate can be prevented by appropriate operation parameters. The work demonstrated the potential of developing reactive crystallization as a technology to deliver phosphorus products with the desired and reproducible quality, and thus to establish long-term phosphorus phosphorus supply with high recycling rate.

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Time-optimal Operation of Diafiltration Processes in the Presence of Fouling

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Membrane separation processes are mainly used for separation of two or more components in a solution. They have found applications in many industries. Separation is achieved due to molecular size differences of the individual solutes. The diafiltration process is designed to increase the concentration of the macro-solute (high-molecular weight component) and to simultaneously decrease the concentration of the micro-solute (low-molecular weight component) to certain specified values. The concentration of the solutes during the run of the process can be influenced by adding a solute-free solvent (diluant) into the feed tank. In our previous work (Jelemenský, 2014) we concentrated on effects of fouling on membrane and we proposed time-optimal operation of diafiltration process. We assumed that fouling influences available membrane area. This paper extends the findings using different fouling models assuming that permeate flux decreases. Several models described in the literature (Hermia, 1982) are studied. These include complete, intermediate, standard blocking models, and cake formation model. We apply methodology of optimal control and use both analytical methods (Pontryagin's minimum principle) and numerical methods (control vector parametrization). The goal is to find properties of the optimal process behaviour and to propose a general feedback control strategy that will cope with fouling. Selected case studies from literature highlight the approach and its properties.

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[293]

Supercritical gas recycle analysis for surge control of centrifugal compressors

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The compression of carbon dioxide for transportation and storage has progressively increased in recent years. This is due to its importance within carbon capture and storage technology, where large-scale transportation via pipeline network is suggested.

In order to increase the gas density while reducing the pressure drop along the pipeline, the gas is compressed to supercritical phase. In order to do so, centrifugal compressors are the most suitable machines due to their operating range. Usually a series of compressors is necessary in order to achieve the needed pressure ratio. The supercritical transition takes place in the last compressor. However, practical problems can arise in the operation of such a compressor, especially when dealing with gas recycle for antisurge protection.

There is a gap in the literature on the effect of dealing with supercritical fluid while controlling a centrifugal compressor. The thermodynamic properties of CO2 change when the fluid enters the supercritical region. Some studies have been conducted regarding the performance of compressors in this area, however there has been little work regarding the control system and the effect of dealing with high density fluid. Of particular interest is the antisurge recycle system because the transition from supercritical to subcritical phase takes place along the recycle line when the antisurge valve opens. The amount of gas recycled is crucial for surge protection and it depends on the temperature and pressure of the gas. Prior work on transcritical CO2 compression operation is found from other research areas such as refrigeration plants and power generation based on a supercritical CO2 Brayton cycle. However in the refrigeration industry the research goal is the thermal optimization of the cycle. Reciprocating and positive displacement machines are used due to their operating range and therefore surge is not a problem. On the other hand, technology involving rotating dynamic compressors, such as power generation based on a supercritical CO2 gas turbine, is still in the early stage of development. Therefore in the future it will need a suitable control system able to deal with the recycle of supercritical CO2.

This paper reports on the analysis and design of control systems for centrifugal compressors when the operating fluid is supercritical CO2. It demonstrates that the design of the control system of the compressor must take into account the state of the fluid. It also evaluates if the plant configuration allows compressor operation within a given surge margin. In order to do so, a fully validated non-linear dynamic model was developed in order to simulate the operation of the compressor at full and partial load. The model includes a main process line with the compressor and also a recycle line with gas cooler and antisurge valve. A control system is implemented in order to control the outlet pressure of the machine while protecting it from surge by means of gas recycle. Boundary disturbances were run in order to show their effect on the compression system and especially on the recycle line. Transient operations are simulated at various recycle temperatures in order to show the effect of this variable on the energy requirement of the process under multiple scenarios. The results show the impact of the operating conditions of the compression station on surge prevention and also their effect on the energy consumption, suggesting better ways of dealing with supercritical fluid while controlling a compressor.

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Software sensors design and selection for the production of biodiesel from grease trap wastes

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In this paper, a couple of software sensors were designed as a monitoring tools for the esterification of grease trap wastes which is a kind of low quality feedstock for biodiesel production. This esterification process has been conducted within a jacketed Continuous Stirred Tank Reactor (CSTR) and both software sensors were designed for the reconstruction of the concentration of Free Fatty Acids (FFAs) from discrete CSTR's temperature measurements. One of these software sensors, called asymptotic observer, is recognized for its capacity to provide estimates without the knowledge of the process kinetics. It has been also designed an estimation algorithm known as reset fuzzy observer. This approach has been recently proposed and is able to update the estimated states at each instant when continuous or discrete measurements are available. Both observers were built regarding the structure of a validated dynamical model for the esterification of grease trap wastes and they were tested considering experimental data. The results show that the asymptotic observer offers a very poor performance when some process's disturbances (e.g. input concentration of FFAs, jacket temperature) are carried out, whereas the reset fuzzy observer is able to reconstruct satisfactorily the concentration of FFAs in the presence of such disturbances. Therefore, this fuzzy observer can be selected as reliable monitoring approach that could be further used as a key part of robust control schemes conceived for this specific biodiesel production process.

[352]

Optimised Operation of a Decentralized Wastewater Treatment Plant with Advanced Nitrogen Removal in the Presence of Online Sensor Failures

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The main objective for controlling the wastewater treatment process is to optimize the operation in order to minimize running costs and to improve the robustness of treatment performance, despite inlet disturbances and possible instrument faults affecting the process. Biological nitrogen removal from municipal wastewater is becoming an increasingly important issue as regulatory pressure increases to limit the levels of nitrogen in treated wastewater discharged in the environment. Wastewater aeration is one of the most energy intensive operations in the treatment process. It is thus essential that an efficient management of oxygen supply is adopted, to guarantee the sustainability of this operation. An intermittently aerated process allows nitrification and denitrification to proceed in the same tank, and this is often the strategy adopted in small scale activated sludge plants such as those operated in decentralized wastewater management systems.

A simulation-based study for the evaluation of the design of aeration cycles for the energy efficient, real time control of nitrogen removal in a decentralized wastewater treatment plant (WWTP) is presented. Options are also presented for keeping process control running even in the presence of catastrophic sensor failures in the inlet ammonia nitrogen and chemical oxygen demand (COD) measurements. Computer simulations have been carried out in a model based framework for performance monitoring, supervision and control specifically adapted to small-scale, decentralized WWTPs. This framework makes use of online data acquisition integrated in a dynamic model structure to manage the bioreactor aeration regime using model-based predictive control. This model-based control depends on a sufficiently accurate mechanistic nonlinear dynamic model of the WWTP developed in gPROMS and comprises three modules: hydrodynamic model; biological treatment description based on the ASM1 model; and suspended solids separation model using a simplified description of a gravity settler. The model has been calibrated and validated with data collected through a series of operational campaigns carried out at a small-scale WWTP treating domestic wastewater, located near Lisbon, Portugal. Simulated dissolved oxygen profiles generated by the dynamic model fed with the obtained input data have been used to test the model performance by comparing them to values measured in the aeration basins.

Dynamic simulations have been used to predict the plant's nitrogen removal ability and propose optimal ranges for aeration management control, under different scenarios of biomass management (sludge age control). This optimization aimed to minimize aeration costs while keeping treatment levels within imposed standards compatible with discharge regulations. These simulation studies indicate that optimal intermittent aeration profiles could be implemented in this type of activated sludge process, providing effective and consistent organic load and nitrogen removal levels and a reduction of energy requirements even in the presence of the tested sensor faults.

[357]

Improving Data Reliability for Process Monitoring with Fuzzy Outlier Detection

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To implement on-line process monitoring techniques that utilize principal component analysis (PCA) or partial least squares (PLS) models, it is important to use reliable data that represents normal process operation when constructing the models. Outliers in data may arise from mechanical faults, changes in system behavior, instrument error, or simply through human error. The contaminating effect of outliers degrades the performance of process monitoring techniques. Therefore outlier detection is used to detect and, when appropriate, remove anomalous entries from process data to improve their reliability for process monitoring. Several outlier detection methods have been investigated but they rely solely on statistical tests to perform a screening of a data set. These conventional methods are often rigid and sometime face limitations posed by their statistical nature.

In this paper, a novel flexible fuzzy treatment method is developed for the detection of outliers in process data. This method utilizes a combination of fuzzy C-means clustering algorithm to separate the data into clusters and a fuzzy inference engine to assign a degree of outlier to data points. The fuzzy inference engine performs an evaluation based on Mahalanobis distance and expert's uncertainty to determine the degree of outlier. This method can be considered a hybrid method that incorporates statistical parameters into a fuzzy strategy. Decisions on how to handle the data can then be made based on the degree of outlier. This degree of outlier can also be conveniently translated into a relative weight assigned to an outlier entering downstream data processes.

The fuzzy treatment method was applied to benchmark penicillin production process data containing outliers data points. The proposed method was able to detect the outliers in the process data with the added advantage of being able to account for an expert's uncertainty in the data. Additionally it is possible to modify the fuzzy inference engine to utilize different criteria, such as data density or spread to evaluate outlierness. The result is presented along with a discussion on the advantages of this method as a flexible treatment of process data. The methodology will be applied to future investigation on PCA based process monitoring.

[368]

Inversion-based Feedforward control design for the Droop model

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An inversion-based feedforward control for the Droop model for microalgae growth in the chemostat is presented. For this purpose the dilution rate is considered as input and the biomass output trajectory is designed for operating point change in given time.

The inversion-based Feedforward design technique is applied, exploiting the asymptotic stability of the two-dimensional internal dynamics (nutrient quota and extracelular concentration) for conditions which prevent an undesired washout attractor.

Numerical results show that the transition time can be significantly reduced by the proposed approach in comparison to a simple step change in the feed flow. The impact of feed substrate changes on the controller performance are numerically evaluated for worst case scenarios, delimiting the possible downgrade due to step changes in this exogenous variable.

[384]

Dynamic Modeling of Pectin Extraction for Monitoring and Optimisation

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Pectin is a family of complex pectic polysaccharides in which the main active chain is the galacturonic acid. Pectin is used as an additive in many foodand pharmaceutical products to modify the rheological properties of the product. Pectin can be used as gelling agent, stabilizer or emulsifier. Pectin can be extracted from different natural sources since it is found in cell walls of plants [1]. At industrial level pectin can be extracted from for instance peels of citrus fruits. Pectin in its natural form is dispersed in the solid phase (peel) and is leached most commonly by acid hydrolysis and then recovered by precipitation with alcohol [2]. Commercial pectin extraction is a batch operation with several tanks that can feed continuously the downstream processing. The variability of the raw material is a challenge because this is a continuous input of uncontrolled disturbances to the process. Consequently, the process conditions should be constantly adjusted in order to obtain not only a high pectin yield but also to ensure good product quality. The pectin quality can be characterized by the degree of esterification (%DE) and intrinsic viscosity (IV) [3]. However the target values of these can change depending onthe product application. Continuous monitoring of these two quality measurements can provide the required information to calculate and adjust the extraction conditions, i.e. amount of peel or pH in order to obtain the optimal pectin quality for the available raw material. Some of the measurements related to the pectin quality can only be carried out when the pectin is in the solid form. This means that the sample is taken after the precipitation with alcohol. The process can take several hours from the extraction to the precipitation. This induces a significant delay in the adjustments of the process conditions. As a consequence, some batches are processed under non-optimal conditions reducing pectin quality. Therefore it would be beneficial to achieve real time process monitoring by coupling available process data to a simulation model and thereby getting on-line predictions of the process output. In that way the process conditions can be adjusted to achieve the optimal pectin yield and quality already during the first batch extraction. In this work, a dynamic mathematical model of the pectin extraction is developed. The purpose of the model is to predict the extraction process behaviour in large scale operation. The model consists of a system of differential equations that describes fundamental phenomena involving chemical reactions and mass transport. The system of differential equations is solved numerically. From the model output guidelines can be obtained to which measurements are needed for an effective monitoring scheme in order to optimise the production.

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[400]

Effect of Solvent Content on Controllability of Extractive Distillation Columns

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The question of a well designed extractive distillation system has been the subject of several works involving all obstacles in the search for design and optimal operation point, which usually involves repeated simulations with large number of results to be analyzed separately. Thus, the findings are limited because the main decision variables, reflux ratio, solvent flowrate and size of the extractive section are not analyzed simultaneously. This article arose from a new approach to evaluating separation and energy consumption of extractive distillation columns using as primary analysis parameter the solvent content throughout the column, more specifically, at the solvent feed stage. The use of this parameter allowed to find a range of possible solutions that will necessarily contemplate the global optimal point of operation, as well as eliminating the obstacles intrinsic to the methodology analysis previously found in the literature, for the extractive distillation process. Based on these results, it was observed that the operating point with a higher solvent content in the extractive section provides considerably better performance, in addition, it was found that the energy consumption of the reboiler of the extractive column is strongly dependent on the solvent content throughout the column. The results also indicate that increasing the solvent content means that the energy consumption becomes independent of the number of stages of the column. However, most of the simulations that did not achieve convergence, because they did not meet specifications, were mainly in the extractive distillation column with fewer number of stages, which lead us to conclude that the column with a higher number of stages presents more options regarding to operational conditions. And that is an essensial information to the design of the process control system. For control purposes, the solvent content required throughout the column may be obtained by the simultaneous manipulation of the reflux ratio and solvent feed flowrate (manipulated variables). In view of this, the design of the control system is the subject of this research and one of the issues that should be investigated is the influence of the solvent content on the controllability of the process. More specifically, this research aims to answer the following question: Is a column with a higher number of stages operating with lower solvent content easier to control than a column with fewer stages operating with higher solvent content? The production of anhydrous ethanol by extractive distillation using ethylene glycol as solvent was used as a case study for this work.

[410]

High purity, high recovery, multi-component methanol distillation control

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High purity distillation is a well-established area of research. In an industrial setting most columns are operated at high recovery rate due to the financial incentives. However, most research work in this area overlooks high recovery. In high-purity (<10ppm) multi-component methanol distillation the columns are usually operated at 97.5% recovery. Increasing this recovery even by 1% carries a significant financial incentive. However, plants operated at higher recoveries frequently encounter controllability issues. In this work a validated model of a methanol distillation column was built in a commercial process simulator and used to study the dynamic behaviour of a real column operating at 97.5 and 99.5% recovery levels. The results showed that at 99.5% recovery minor deviations in product draw rate and feed flow have a significant impact on column operations and exhibits highly nonlinear behaviour in comparison to 97.5% recovery. The analysis also showed that exceeding 100% methanol recovery for long durations leads to poor long term column control. Based on the analysis the following novel predictive control scheme has been developed and tested for 99.5% recovery: The predictive control scheme extracts flow and composition information from feed, product and side draw streams to dynamically calculate the mass and energy requirements. The information is then used to set reboiler duty, and to manipulate the set points of the decentralized product ethanol composition controller and side draw flow controller. These actions manage the energy requirement, methanol and ethanol mass balances respectively.

[417]

Implementation of Model Predictive Control in Industrial Gasoline Desulfurization Process

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Sulfur is an important pollutant in transportation sector. It can severely prevent an implementation of all major pollution control strategies. Thus, to reduce air pollution and to comply with strict environmental regulations, sulfur content in all types of fuel produced is required to be lowered to a certain level. With Euro IV specifications, a maximum of 50 ppm of sulfur in gasoline is required.

In one oil refinery in Thailand, a selective desulfurization unit was installed to significantly reduce the sulfur content of fluidized catalytic cracked (FCC) gasoline. This unit consists of three major units including selective hydrogenation unit, FCC-gasoline splitter unit, and hydrodesulfurization unit. Though, the desulfurization unit can considerably lower the sulfur content of the gasoline. Some undesirable olefin saturation reactions occurred, resulting in octane loss of the gasoline product. The octane loss depressingly influences economic performances of the plant. Thus, optimizing the operation in order to minimize the octane loss while still complying with sulfur specification and other process constraints is necessary. The operation optimization can be accomplished by implementing model predictive control (MPC).

In this work, we focus on the implementation of MPC in the selective hydrogenation unit in order to strictly control sulfur content in the gasoline product while minimizing octane loss. A soft-sensor for on-line estimating sulfur content in gasoline product was designed and implemented. A series of step tests were performed to build empirical dynamic models. The models obtained were validated and used in MPC design. Analysis of benefit was performed with data collected before and after MPC implementation. The results showed that after MPC implementation, the control performances were improved by shifting mean of the sulfur content in product close to the high limit operation. Thus, energy consumption was significantly decreased.

[443]

Maximizing Profit of Semi Batch Autocatalytic Esterification Process in the Presence of Disturbance: Application of Cascaded-Conditional Based Online Dynamic Optimization

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In semi batch esterification process, a disturbance such as variation concentration in the feed stream may cause the final product differs from the desired value. This discrepancy may risk the violation of safety constraints, production off-spec products, and more vitally the loss of invaluable profit. Under these circumstances it is desirable to implement online dynamic optimization strategy to desired trajectories to reach the optimal performances. In cascaded-online dynamic optimization, the overall problem is decomposed into two sub-problems (with consistent objectives) that need to be subsequently re-integrated in closed-loop. The set-point trajectory that guarantees performance is computed. A `low level' tracking controller ensures that the system does not deviate from the optimal trajectory. In addition, a `high level' optimizer is invoked periodically to ensure optimality despite disturbances. The cascade optimization approach combines the positive features of optimal operation and feedback control. Based on the trigger system (activation re-optimizer), it is preferred to apply conditional-based optimization with no repetitive update. Due to disturbance, pre-determined optimal trajectories need to be updated but it may not be necessary as the updated solution and the predicted benefits (objective function) may not be significantly different from the reference solution. Consequently, conditional-based optimization can be implemented which initiate a solution of the dynamic optimization problem only if necessary; otherwise it follows pre-determined optimal trajectories

This work addresses the implementation of an online dynamic optimization cascaded with a dual mode PID control strategy for improving the product quality and profit of an autocatalytic esterification of Propionic Anhydride with 2-Butanol. An orthogonal collocation method is implemented to re-optimize the feed rate and temperature trajectories to compensate the deviation of end product due to disturbance (variation of feed concentration). The problem of dynamic optimization is formulated to maximize the profit. The spec of final product (±5% of conversion) constraint is denoted as an active constraint which is applied as the trigger for activating re-optimization. The simulation results show that the proposed strategy offers a large improvement in semi batch reactor performance if compared to the method which the optimal trajectories set point is pre-determined (offline). Moreover, the online dynamic optimization of temperature and feed flowrate trajectories obtained able to sustain the limiting reactant concentration within active constraint. Meanwhile, the offline optimization failed to handle the effect of disturbance thus the end concentration produced is off-spec and can lead to loss in profit.

[459]

MIMO Neural Wiener Based Model Predictive Control (NWMPC) For MTBE Reactive Distillation Using Simulated Annealing- Particle Swarm optimization (SA-PSO)

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MTBE is commonly produced using reactive distillation column which combine reactor and distillation column in single unit process. To achieve high MTBE purity and reactant conversion is a challenging task due to strong interaction between control variables and highly nonlinear process. In this work, nonlinear model predictive control (NMPC) was developed and applied to control tray temperature of MTBE reactive distillation. Tray temperature is proposed in this work because it can be correlated to MTBE purity. To increase the performance of NMPC, the Neural Wiener model and Simulated Annealing –Particle swarm optimization (SA-PSO) were chosen to be implemented in NMPC. Neural wiener is one of block oriented model which can produce good modeling capability with less computational time. Meanwhile, combination of SA-PSO will increase accuracy of the controller optimization. PSO has a strong ability finding the most optimistic result but weak to find in local minimum. This PSO algorithm was combined with SA optimizer which has a strong ability finding the local optimistic result but its ability finding the global optimistic result is weak. In this work, the MTBE reactive distillation was modelled using aspen dynamic, meanwhile the control study has been simulated using Simulink (Matlab) which is connected with Aspen dynamic model. The results obtained show that the multi input multi output (MIMO) Neural Wiener based model predictive control (NWMPC) using SA-PSO was successfully applied to control tray temperatures in MTBE reactive distillation. The NWMPC proposed was able to track set point, reject the disturbances very well with small value of error. The robustness test also shows that NWMPC is robust towards uncertainties of the process.

[460]

Online models for increased plant availability

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Chemical production plants today are generally planned with the help of process models based on steady-state simulators. Besides commercial simulation tools from ASPEN, Bayer AG also uses VTPLAN, a proprietary, equation-oriented simulator for steady-state processes. The models are stored in model library.

One of the things driving the trend toward ever-larger plants is the need to increase their availability and avoid unscheduled downtime. Detailed monitoring of critical plant components (equipment performance monitoring) is absolutely essential for achieving these objectives. Thermodynamic computations are generally required to identify these "soft sensors."

The development of an additional interface between VTPLAN and the process data archive enables existing process models to be operated online. Roughly 40 online models are currently in use at Bayer AG, including models of complete plants, individual plant sections and models of cross-plant utility systems.

This presentation uses selected examples to illustrate how online models can increase the availability of large-scale plants and lead to better process understanding.

[470]

Energy Optimization in Pasteurization Processes

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Within many industry sectors drying, evaporating and heating are the most energy demanding processes, with limited technical opportunities for energy recovery. Besides their non-linearity, these processes are complex in terms of control design since their system dynamics require fast control cycles. For this work, the pasteurization process of bottled or canned liquid products is investigated. Its high energy demand occurs due to hygienic issues. For the products, the heat treatment is done in large scale equipment, so called tunnel pasteurizers. These plants are tunneled conveyer belts that are sprinkled with hot water for heating whilst cold water is used for re-cooling the products. The presented approach was realized for a tunnel pasteurizer with 18 coupled heating/cooling zones. From the process point of view, it is a complex combination of multiple coupled heat transfer systems with constraints. From the mathematical point of view, it is a distributed parameter system that can be described using a Partial Differential Equation (PDE). In general this model identification is a crucial point since it might be very time and costs demanding in order to achieve an acceptable result for online optimization applications e.g.: within an model predictive controller (MPC). The model of the pasteurizer has to cover the parameters like conveyer speed, zone temperature, product temperature at inlet, temperature of environment, and their impacts on the quality parameters like pasteurization units (PU) and time above temperature (TAT). A modeling approach, where the process is described by PDEs, is set up and for the numerical solution the implicit Crank Nicolson scheme, as well as the explicit Euler approach are considered. For Crank Nicholson guaranteed numerical stability is applied. Furthermore the approach transfers the PDEs, with high accuracy, into a state space model. The design of the PDE includes several additive terms, describing the diffusion of the heat between products, the number of heating / re-cooling zones, the impact of the water spray temperature in the different zones on products and the heat losses to the environment. To transform PDEs into State Space Models used within an MPC the discretization in conveyor direction is set to 50 steps, representing one meter of the physical plant length. The discretization in time is varied between 0,05 and 0,5 seconds. The implicit Crank Nicholson scheme delivers more robust and accurate results for larger discretization steps compared to explicit Euler approach, which is becoming unstable solving the PDEs numerically. The shown approach delivers good results for online optimization of distributed parameter systems, representable as parabolic PDEs. Applying Crank Nicholson for discretization of the PDEs delivers State Space Models with high mathematical accuracy. The use of these State Space Models within the framework of MPC allows the application of both Input- and Output-constraints and guarantees low calculation load needed for online closed loop control.

[505]

A real time particle size control framework in non-isothermal antisolvent crystallization processes

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Crystallization is one of the main processes in industry that occurs as a result of changes in solubility equilibrium, and is widely used for solid-liquid separation. Today various sections of the chemical industry, at some stages, utilize crystallization as a method of production, purification or recovery of material. A tight control of the Crystal Size Distribution, CSD, are commonly required in the production line as it can largely influence the textural and physical properties of the final commercial products such as filtration and dissolution rate.

This contribution presents an online strategy to directly control CSD in joint cooling antisolvent crystallization operation. The proposed methodology involves the use of a novel stochastic formulation, the Fokker-Planck equation (FPE), as model to represent the time evolution of the particle characteristics, and for off-line determination of optimal trajectories in terms of manipulated parameters (temperature and antisolvent feed rate) and controlled variables (mean size and standard deviation). A map of iso-mean and iso-standard deviation curves are used in an antisolvent flow rate-temperature plane based on evaluating the model at asymptotic condition. This allows selecting the reachable CSD characterized by mean and standard deviation. In order to monitor crystals' features, digital image texturing analysis approach is discussed and implemented, providing the on-line information for further feedback control action. Taking advantage of image analysis as an in situ technique of data sampling, crystals' characteristics can be measured in real time and a feedback control loop is achievable. Alternative control configurations are implemented and tested to attain a desired CSD. They include multi-loop PIDs approach, a feedforward strategy based on off-line calculated profiles and a two stages control structure using a combination of feedforward and model-based feedback algorithm. Results demonstrate a poor performance of the PIDs control strategy, due to ill-conditioning nature of the process. On the other hand good behavior on the mean size control is achieved when the proposed two stages controller is applied. Experimental validation of the strategies is carried out for the ternary system of water-ethanol-sodium chloride.

[520]

Proposal of a New Pathway for Microalgal Oil Production and its Comparison with Conventional Methods

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Growth of microalgae on commercial scale for production of fuels or fuel based chemicals needs large amounts of nitrogen and phosphorus fertilizers as nutrients. Production of nitrogen fertilizers consumes vast amount of energy from fossil resources and generates greenhouse gas emissions. Phosphorus resources are also finite in nature. Therefore, the use of these fertilizers is one of the major constraints for energetically feasible and sustainable production of fuel from microalgae at commercial scale. In a recent biological study, a distinct species of microalgae, Botryococcus braunii, which can produce the long chain hydrocarbons and excrete them outside of the cell wall, has been tested for repetitive extraction of its hydrocarbons - termed as milking. The determination of the ability of the Botryococcus braunii to produce the hydrocarbons repeatedly without any extra supply of nutrients is expected to be an important step towards the sustainable production of fuels and chemicals from microalgae.

In this study, the newly proposed method has been compared with the conventional method for the growth of microalgae to produce similar amount of microalgal oil. The mathematical models consisting of mass balance equations were developed using Aspen Custom Modeler for both the conventional microalgal growth system and the process of repetitive production of hydrocarbons from Botryococcus braunii. The amount of micoalgal oil/hydrocarbons to be produced was taken as the basis. The biological parameters such as productivity and oil contents of microalgae, concentration of algal biomass in culture media, number of days required for repeated production of hydrocarbons and number of repetitions up to which Botryococcus braunii is able to produce the hydrocarbons are the inputs to the model. Nitrogen fertilizer, phosphorus fertilizer, water and CO2 requirements have been calculated for both the conventional and milking systems. The area required for growth of algae in both these systems has also been calculated using the model. Using the outputs from material balance equations together with the assumptions taken from literature for energy consumption, the direct and indirect energy requirements for paddle wheel mixing, water pumping, fertilizer supply and CO2 supply have also been calculated.

The results show that compared to the conventional system, the fertilizer requirement, water consumption and energy inputs in the milking process can be decreased up to 90%, 60% and 50%, respectively, by using the milking process. This shows that the milking system has the potential to reduce the overall energy input to the process of production of fuel from microalgae. Also, high heating value of hydrocarbon contents of Botryococcus braunii gives the higher energy output resulting in higher output to input energy ratio of the process, making it energetically more feasible than the conventional system.

[535]

Multivariable Adaptive Lyapunov Fuzzy Controller for pH neutralisation process

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A multivariable fuzzy logic controller with Lyapunov adaptive control scheme has been developed for a pH neutralisation process. In this study, the nominal neutralisation process condition exhibit the nonlinear dynamics and multi-delayed-effects input variables. The proposed controller uses a Takagi-Sugeno fuzzy inference system and it has been optimised by using input-output data sets obtaining from experimental of synthetic waste water titration. The genetic algorithm is used to train the multi-inputs-multi-output fuzzy structures and the optimised structure is used to predict three difference control action simultaneously. The Lyapunov function is implemented to modify the fuzzy inference at every output membership function and it will minimizes the error. The proposed controller has been tested and compared in several cases such as for set-point tracking, model plant mismatch and unknown disturbance. The adaptive fuzzy controller demonstrate better performance over the conventional PID controller in all tested cases.

[560]

Detection of changes in fouling behaviour by simultaneous monitoring of thermal and hydraulic performance of refinery heat exchangers

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Monitoring of pre-heat trains efficiency in oil refineries is a crucial practice to evaluate the gradual decay in performance of heat transfer equipment due to fouling and assist in operational decisions in respect of fouling mitigation options and cleaning actions. Typical refinery monitoring techniques focus on assessing the thermal performance of heat exchangers by calculating fouling resistances using temperature measurements. However, looking only at the thermal performance of a heat exchanger – or a heat exchanger network – only tells part of the story and plants exist where hydraulic issues (i.e. excessive pressure drops generated by the gradual build-up of fouling inside the tubes) are dominating over thermal ones. Current practices not only ignore the hydraulic performance, but also have limited capabilities to highlight changes in the fouling behaviour. In this paper, a novel graphical representation of time varying operational data is proposed to monitor crude oil fouling based on online plant measurements. This representation simultaneously captures the thermal and hydraulic performance in a way easily interpreted by engineers.

A recently developed model for the description of the fouling process, which permits incorporating (and evidencing) subtle changes in fouling behaviour, is implemented in a shell-and-tube heat exchanger framework (Coletti and Macchietto, 2011). It is shown that the resulting model can capture the different thermal-hydraulic behaviour experienced in industrial systems undergoing distinct types and rates of fouling. This is shown first for controlled inlet conditions of temperature and mass flowrate (to simulate situations arising from, say, a change of crude), and then for actual (time-varying) measured inputs from a refinery. It is shown that this monitoring approach is useful to: a) simultaneously evaluate and trend the interacting thermal and hydraulic performance over time; b) detect deviations from the expected performance due to change in fouling behaviour; c) help in the identification of different types of potential fouling causes. The results show that consideration of both thermal and hydraulic effects is essential to adequately detect changes in fouling behaviour merely based on measurements of inlet and outlet streams to heat exchangers, and highlight the capabilities of the approach presented to monitor the performance of heat transfer equipment undergoing fouling under industrially relevant conditions.

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Dosage of Filter Aids in the Case of Pure Surface Filtration – An Optimal Control Approach

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Filter-aid filtration is widely used to remove impurities which would otherwise clog the filter medium. Due to its flexibility concerning the separation task, it is applied in a whole range of fields, such as in the biotechnology and chemical industry, in water treatment and the production of food and beverages. Important decisions, hereby, are how much filter aid to add and when to add it over the course of the process in order to minimize the filter cake resistance, i.e. energy expenditure, while consuming a minimum amount of filter aid. These decisions are usually made solely based on simple rules derived from practical experiences.

For a more rigorous treatment, we adapted a model from the literature which represents cake resistance as exponentially depended on the ratio of impurities and added filter aid. It was derived for the case of pure surface filtration and has been validated several times. This approach is reformulated so that it holds for the local filter-cake properties and is coupled with an incompressible cake-filtration model for variable solid concentration in the liquid phase. The filter-aid dosage is subsequently expressed as an optimal control problem and solved with the calculus of variations. This is the first application of optimal control theory to filter-aid filtration and among the few concerning filtration in general.

The first finding is that in case of a constant impurity concentration in the liquid, the optimal strategy for a minimum filter-cake resistance is a constant dosage of filter aid. Furthermore, the optimal filter-aid dosage trajectory in case of a time-variable impurity concentration is derived. Numerical studies of different dosage trajectories are shown which also proof that the extrema found are indeed optima.

Trivial, as the first result may initially sound, especially its negative implications are far-reaching. If, under the consideration of pure surface filtration, constant dosage is optimal, then clearly a constant filter-aid dosage is no longer optimal when depth filtration also plays a significant role – which is indeed the case in many applications of filter-aid filtration. However, in industrial practice filter aid is mostly dosed constantly. The results to be presented, therefore, give a concise mathematical argument that the development and implementation of more sophisticated dosage strategies are beneficial.

[595]

Best of Breed control of batch precipitation reactors

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Batch reactors are very important to the refining process of platinum group metals and their effective control is essential to ensure safe and efficient process in minerals industry (Singh et al. 2010). In these reactors various process phases are encountered in a single process batch; they could be heating, cooling and reaction phase. These reactions occur as either an exothermic or endothermic reaction and the control of the batch reactors is essentially treated as a temperature control problem (Friedrich and Perne, 1996). A change from one batch to another batch could necessitate a change in control actions and this makes the control more difficult as different models are applicable for different batch process recipes operating at different operating conditions (Singh et al. 2010). The temperature control of the reactor is carried out with PID controllers in a cascade structure in many industries, a good temperature control is hard to achieve with these controllers (Stampar et al. 2013). The use of advanced process control (APC) systems has the potential to improve the control of batch reactors employed in the refining process of PGM's (platinum group metals) (Singh et al. 2010). An existing batch precipitation reactor in the mining industry was modelled from first principles using MATLAB S-function language and wrapped into Simulink custom blocks. The model was validated with open loop simulations to evaluate the response to step changes in the model inputs. Two PID controllers with different parameters were implemented on the model at different operating points and their temperature control performance was evaluated based on their ability track a temperature of the industrial reactor as a set-point. The performance of the controllers was measured and compared using an integral time-domain performance measure. A commercial advanced process controller (APC) was implemented on the model, a communication interface between the model in Simulink and the commercial controller was developed with Industrial Data Xchange (IDX); an OPC client and server. PID controllers perform better on model operating points there were tuned on with a lower integral square error (ISE) and their performance degrades with change in process operating points and batches (Noguchi and Kobari, 2005). To overcome these limitations, a commercial APC (Aspen DMC Plus) which has been successfully connected to the Simulink model will be completely implemented to validate (Singh et al. 2010)'s work on the actual commercial reactors which proves that the APC controller out-performs PID controller. The platform needed to compare ability of the PID and the APC control system with the reactor model was developed.

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Multivariate analysis of industrial scale fermentation data

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Batch production processes pose specific challenges for process monitoring and control. This is due to many reasons including non-linear behaviour, and a relatively poor understanding of the system dynamics [1]. It is therefore challenging for the process engineer to optimise the operation conditions, due to a lack of available process models, and complex interactions between variables which are not easy to define, especially across scales and equipment. There is however a vast amount of batch process data generated, which can be investigated with the aim of identifying desirable process operating conditions, and therefore areas of focus for optimising the process operation. This requires multivariate methods which can utilise the complex datasets which are routinely collected, containing online measured variables and offline sample data.

Fermentation processes are highly sensitive to operational changes, as well as between batch variations, and are therefore an interesting application of multivariate methods. The process dynamics are governed by the combination of process variables, and cannot be fully characterised by individual variables alone [2]. There is also a lack of sensors for key variables which are considered to define the operation [3], which makes traditional modelling a challenge.

Although multivariate techniques are routinely used for chemometric applications, their application to batch processes is less common due to the additional challenges associated with uneven batch lengths and less reproducible data, which has naturally greater variability, as well as high measurement noise. This requires additional preprocessing stages in order to extract the information within such a dataset.

A 30 batch dataset from a production process operating at Novozymes A/S is analysed by multivariate analysis with the aim of predicting the final product concentration, which is measured offline at the end of each batch. By creating a model for product concentration, it is possible to analyse the model results and interpret this to guide process optimisation efforts towards achieving a greater product concentration.

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Model-based Observation and Design of Crystal Shapes via Controlled Growth-Dissolution Cycles

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Control of multivariate population balance systems is a challenging task in process engineering, which is in particular due to difficulties in observing the state of the dispersed phase. In this article, we present a setup based on video microscopy and Kalman filtering to observe the evolution of a crystal population in batch crystallization processes. We demonstrate the applicability of our methods on the cyclic batch crystallization of potassium dihydrogen phosphate. It is shown that the cyclic process strategy can lead to crystal shapes which would not have been attainable via pure growth processes.

[608]

Adsorption based competitive purity control in crystallization

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Crystallization of active ingredients and fine chemical products, which are contaminated by undesired impurities (e.g. genotoxic impurity) originated from upstream processes can be a critical challenge in pharmaceutical, food and fine chemical production. Adsorption based purification techniques for liquids, especially waste water treatment is widely researched. Similarly the effects of impurities on the crystal properties such as crystal shape or effectiveness of the crystal for solvent based purification is also studied, while adsorption based purification of crystal product has not been investigated jet [1,2,3]. In this work an adsorption-based growth model is used in conjunction with the population balance model, to describe the effect of multiple impurities on the crystallization. The model is able to simulate the composition of the crystal lattice during crystallization in impure media taking into account the competitive adsorption of multiple impurities. Based on this model a Competitive Purity Control (CPC) is proposed, which can be a suitable technique in order to lower or eliminate the non-desired impurity from the solid crystal product.

The mathematical model based on morphological population balance and extended crystal growth kinetic equations which can describe the adsorption mechanism is used to investigate and optimize the crystallization process in impure media. Regarding to the competitive adsorption mechanism, non-desired impurity could be lowered by using chemical compound, which adsorbs to the same type of active site on the crystal facet.

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Stabilizing control for reactor/separator processes with gas and liquid recycles

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A reactor/separator process with gas and liquid recycles is one of the most common process configurations in chemical plants. In this paper, a control system design problem for such processes is discussed using the two representative plantwide control benchmark problems, namely HDA (hydrodealkylation of toluene) and VAM (vinyle acetate monomer production) plants.

The most commonly used control configuration for gas and liquid recycle systems is to introduce the gas feed as a pressure controller handle, while the fresh liquid feed is provided as a make-up to the liquid feed inventory. In most cases, a liquid hold-up tank is often implemented, to which the liquid recycle and fresh feed streams are introduced. From the buffer tank, the liquid feed is pumped out to the reactor. The installation of such buffer tanks is most helpful for eliminating the positive feedback effect due to the material recycle and making control system design easy.

However, from the viewpoint of process safety (the concept of inherently safer processes) and other operational reasons, this paper seeks the possibility of eliminating such buffer tanks and configuring a stable control system despite the positive feedback effect. The liquid feed stream to the reactor is put on flow control by manipulating the fresh feed stream: the liquid feed to the reactor is the sum of the fluctuating recycle stream and the fresh feed stream. Locally, configuring a simple mixing control may seem sufficient for such systems, but it is shown that the stability strongly depends on the reaction kinetics and the gas component inventory control: the elimination of the buffer tank results in a open-loop unstable process for the VAM plant example, but an appropriate control scheme, ex. PI control, can easily realize a stable closed-loop system.

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Parameter estimation and concentration inference for an enzymatic hydrolysis reactor

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Cellulose is one of the most abundant components of vegetal biomass that is a linear polymer of β-D-glucose, and by (chemical or enzymatic) hydrolysis reaction may be decomposed into fermentable sugars, which can be used in biorefineries to process products with high added value. Enzymatic processes are capable of yields close to 100% due to improvements in enzyme technology made in recent decades. The research topics relevant to enzymatic processes mainly include understanding the phenomena and process design, the improvement of the basic mechanisms of the hydrolysis reactions, and the development of enzymes for greater efficiency and lower cost [1]. Robust strategies for monitoring and process control are often based on a model, which depends highly on the values of the parameters involved. In particular, the enzymatic reactions are related to the uncertainty in some kinetic terms as they may depend on the type and concentrations of substrates and enzymes, temperature, pH, etc. This makes that variability in the raw material or operating conditions causes changes in the kinetic parameters. The accurate or optimal parameter estimation consists, in practice, in to correctly establish a design of experiments and reduce confidence intervals associated with the estimated parameters. On the other hand, to keep the conversion yields, it is necessary to monitor the concentration of product (i.e. glucose) within a future horizon to correct the process manually or automatically.

In this paper the problem of estimating the kinetic parameters and the inference of the glucose concentration in an enzymatic hydrolysis reaction of cellulose, using Trichoderma reesei as enzyme, is tackled. The batch reaction is carried out in an isothermal experimental reactor, with online acquisition of measurements for temperature and pH, and offline discrete measurements of glucose concentration (measured using a blood glucometer [2], previously calibrated with a biochemical analyzer, YSI). The study considers the effect of the reaction temperature and the experimental validation of reactions at three different temperatures. Two estimation techniques are presented and compared: (a) off-line estimation: the kinetic parameters of the Michaelis-Menten equation [3] are estimated using an optimization problem, which can be used into a model for future reaction simulations; (b) on-line estimation: the kinetic parameters are inferred using a nonlinear state estimator (which is a Luenberger-type observer with resolubility conditions and tuning guidelines [4]), allowing the adjustment of the kinetic parameters in the present and the prediction of the glucose concentration in a future horizon of an hour. The online estimation has great advantages: does not require pre-setting model parameters, adjusts the parameters as the reaction progresses, and predicts the glucose concentration allowing do corrective actions to the process. The results will allow further studies of scaling, optimization, monitoring and control online.

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Extended VRFT Method for Controller Design of Nonlinear Systems Based on Block-Oriented Model Structures

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Most dynamical systems can be better represented by nonlinear models, which are able to describe the global behavior of the system over wide ranges of operating condition. One of the most frequently studied classes of nonlinear models is the block-oriented nonlinear model, which involves a cascade combination of a linear dynamic block and a nonlinear static (memoryless) one. Two typical block-oriented model structures are the Hammerstein and Wiener models. In the Hammerstein structure, the linear dynamic element is preceded by the static nonlinearity. The order of connection is reversed in the Wiener structure. A more general model structure is the Hammerstein-Wiener structure in which the linear dynamic element is placed between two nonlinear static functions. These model structures have been successfully used to describe nonlinear systems in a number of practical applications in the areas of chemical processes, biological processes, signal processing, and control. In the last decades, a considerable amount of research has been carried out on identification and control of the nonlinear systems using the block-oriented representations. Traditional control design approaches are often based on mathematical models that approximate the behavior of the physical process. There are two steps in the model-based controller design: an empirical model of the process is identified first and is subsequently used with certain algorithms to design the controller. The identification process, however, usually relies on some prior assumptions such as model structure and order, which are often unavailable or subject to uncertainties. Hence, the complexity and modeling errors associated with such models increase the difficulty of the control design task, and may lead to degradation of control performance. Data-based control design methods are very useful in many practical control applications, where obtaining a suitable model is a very difficult task. The virtual reference feedback tuning (VRFT) method can be used to design the controller by directly using a set of process data without resorting to process models. Most existing results on the VRFT design are however restricted to linear systems. Although some extensions of VRFT to nonlinear systems have been previously reported, these extended versions of VRFT are no longer one-shot methods so that a significant advantage of VRFT is lost. This study proposes a novel controller design method for nonlinear systems based on three types of block-oriented nonlinear models and the one-shot (noniterative) VRFT design framework. Linearizing control schemes which consist of the inverse of the static nonlinearity and a linear controller is adopted. Basis functions, such as the B-splines, are used to represent the static nonlinearity (or its inverse). Combining the parameterization of the nonlinearity with VRFT framework allows putting the system in linear regressor form, so that least-squares techniques can be used to determine parameters of the nonlinearity and the controller. Distinctive features of the proposed method includes: (1) only process data from one-shot experiment are required for control system design; (2) model identification of the linear dynamic subsystem is not required, whereas only the static nonlinearity has to be estimated; (3) nonlinearity estimation and controller design are performed simultaneously without the needs of nonlinear optimization and iterative procedures. The effectiveness of the proposed controller design method is demonstrated through simulation examples of several benchmark processes, e.g., a binary distillation column, a pH neutralization process, and a fuel cell.

[661]

Influence of the Solvent Content on the Dynamic Behaviour and Controllability of a Thermally Coupled Extractive Distillation Process

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Distillation processes are responsible for a representative share in the energy consumption of a chemical plant. In this sense, several solutions have been announced over the past few years and researches reveal that the use of thermal couplings in conventional distillation sequences results in significant reductions in energy consumption, which can generate savings of up to 30%. In extractive distillation, one of the known configurations is the extractive distillation sequence thermally coupled to a side rectifier (TCEDS-SR). The design of this configuration was obtained using a vapor phase thermal connection between the extractive column and recovery column, which eliminates the reboiler of the second column of the conventional sequence. However, obtaining the optimum design and operation of this sequence faces the same difficulties of a conventional configuration (DS). To circumvent these obstacles, the analysis procedure developed for the DS sequence that includes the solvent content in the extractive section as a parameter of analysis was extended to the TCEDS-SR sequence. In the DS sequence, the use of this parameter allows to find the range of possible solutions that will necessarily contemplate the global optimum point of operation, as it eliminates one of the main problems of extractive distillation optimization: the multiplicity of solutions. The proposed analysis procedure was applied successfully for a TCEDS-SR, determining the global optimum, and also, a post-optimization analysis was performed. In the TCEDS-SR sequence, besides the reflux ratio and solvent flowrate of the extractive column, the steam flowrate in the stream that interconnects the columns should be included in the analysis procedure. The results show that the TCEDS-SR configuration is more attractive from the point of view of economics, as it can achieve a significant reduction in the total annual cost (TAC) and in the specific energy consumption (SEC), compared to the conventional configuration (DS). However, the implementation of thermally coupled columns requires an adequate understanding of the dynamic behavior and control properties. The purpose of this paper is to study the dynamic behavior and analyze the effect of the solvent content on the controllability of the anhydrous ethanol production process using a TCEDS-SR sequence. The control structure was defined using the criteria of sensitivity for determining the temperature control and taking into account the viability of the steam flowrate as a degree of freedom.

[690]

Linear or Nonlinear? Comparing Measures of Nonlinearity

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Nonlinearity has a very significant effect on the - closed loop performance of a process as it can render controller tuning ineffective. Nonlinearities can initiate oscillations in process variables that may cause plantwide oscillations, which in turn results in loss of plant profitability and rapid wear and tear of plant machineries. Thus, quantification of nonlinearity is important for designing appropriate controllers and ensuring smooth operation of a process plant. Two major approaches are generally used for quantifying nonlinearity – 1.Model based methods and 2. Data based methods - The preference of the Data-based approaches over the Model-based resides on the fact that Model-based approaches, like Best Linear Approximation and Curvature-Based methods, require a process model which is often unavailable or difficult to obtain. Therefore, in recent time data based methods are gaining popularity because they require time series data of the process which are readily available from the DCS or data historian. The data-based approaches include bicoherence based approach, surrogate data-based approach, Lyapunov exponents and Correlation Dimension. In this paper, data based methods are compared on a few common processes such as a nonlinear spherical tank, a nonlinear Continuously Stirred Tank Reactor (CSTR) and a pH neutralization process to evaluate their suitability and efficacies. They will also be evaluated using an experimental set-up consisting of a conical tank. Finally, they will be applied to an industrial data sets for judging the adequacy of linear controllers and evaluating the need for a nonlinear controller.

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Model Predictive Control for the Self-Optimized Operation in Wastewater Treatment Plants

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The efficiency of most wastewater treatment plants (WWTP) is an important issue that has still to be improved. In order to fulfil the effluent legal requirements for all weather conditions, which generate large variations of the influent, the operating costs are usually higher than the actually needed. Therefore, the optimization of the WWTP operation can provide a significant cost reduction. For minimizing the economic loss, Real Time Optimization (RTO) techniques can be applied to re-optimize the plant, but as they are usually very demanding computationally, the set point optimization can be performed off-line. In this work, the approach considered is the self-optimizing control (SOC) procedure of Skogestad (2000), which consists of determining some controlled variables (CVs), also called self-optimized variables, that when kept constant, the economic loss is small with respect to costs when the operation is re-optimized. Although there are many successful works of SOC, the dynamic validation of the results isusually performed by means of decentralized PI controllers.The first objective of this work is to find the self-optimized variables in a WWTP as a combination of the available measurements. The second objective is to evaluate the dynamic behavior of those variables by implementing two control structures: a centralized nonlinear multivariable model predictive controller (NMPC) with constraints, for controlling the self-optimized variables and the active constraints, and a distributed control structure with an NMPC controlling the self-optimized variables and local PI controllers for the active constraints control. The methodology has been applied to the activated sludge process using the Benchmark Simulation Model No.1 (BSM1). Moreover, in this work a pre-selection of measurements and combinations of measurements has been performed studying the economic losses for different weather conditions, in order to avoid subsequent infeasibilities in the operation for the obtained CVs.Once the economically optimal CVs have been obtained, their closed loop control dynamic behavior has been evaluated, when typical disturbances are applied to the process. This study is an essential step for a successful implementation of SOC, because the methodology is only based on steady state models. The use of the centralized NMPC is a straightforward solution to control the process because the interactions are automatically tackled by the controller when performs predictions. Nevertheless, the number of tuning parameters is rather high, making the tuning a difficult task. This motivates the search for more simple and robust control structures such as distributed NMPC-PI controllers. The control of active constraints is crucial for the optimal operation of the plant, and this control structure has the advantage that if the NMPC fails, the PI controllers still keep the active constraints in the desired values. In order to select the most appropriate loops for PI control in the decentralized NMPC-PI control structure, the Relative Gain Array (RGA) matrix has been calculated. The PI controller has been tuned following typical SIMC guidelines, with some practical considerations due to the complexity of the process.

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Off-Line Tube-Based Robust Model Predictive Control for Uncertain and Highly Exothermic Polymerization Processes

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Polymerization processes usually contain some uncertain parameters such as those in kinetic rate constants and heat transfer coefficients. An inefficient handling of these uncertain parameters may lead to unexpected thermal runaway of the reaction. In this paper, off-line tube-based robust model predictive control (MPC) is developed. The trajectories of uncertain systems are restricted to lie in a sequence of tubes so robust stability and constraint satisfaction are guaranteed in the presence of both uncertain parameters and disturbances. All of the optimization problems are solved off-line so the proposed algorithm is applicable to fast dynamic polymerization processes. The proposed algorithm is applied to an illustrative example of continuous stirred tank reactor where highly exothermic polymerization reactions occur. The results show that robust stability and constraint satisfaction are guaranteed.

[766]

Optimization Based Constrained Unscented Gaussian Sum Filter

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Constrained state and parameter estimation of nonlinear dynamical systems is important for applications such as process monitoring, optimization and model based control. Nonlinear state estimation using recursive Bayesian estimation generally needs to overcome two challenges: (i) provide an accurate representation of the prior density, which is typically non-Gaussian; and (ii) ensure that the estimates satisfy state constraints. In literature, the widely used Extended Kalman Filter (EKF) and Unscented Kalman Filter (UKF) are based on the simplifying assumption of Gaussian prior. Several other sampling based approaches, such as Particle Filter and Gaussian sum approaches have been developed in literature (Patwardhan et al., 2012) that do not assume Gaussian prior. However, these approaches generally tend to be computationally intensive. A recently developed approach, called Unscented Gaussian Sum Filter (UGSF) approximates the prior using a Gaussian sum approach but at a significantly reduced computational cost relative to existing Gaussian sum approaches (Kottakki et al., 2014). Specifically, the UGSF approach has a similar order of complexity as the UKF, that is, it is based on the Unscented Transformation (UT) which has 2n+1 sigma points, where n represents the state dimension. The reduced computation cost is made possible through a judicious choice of various design parameters in the Gaussian sum framework. Several examples have demonstrated the benefit of UGSF over UKF as well as the GS-UKF approaches (Kottakki et al., 2014). However, the UGSF does not incorporate any constraints while estimating the states and thus, may not result in meaningful estimates when the true states are close to the constraints.

In this work, we propose to extend the UGSF approach to incorporate constraints on states. This is achieved by replacing the update step of UGSF by an optimization formulation that incorporates various state constraints. The optimization formulation can be viewed as a Gaussian sum extension of that proposed by Vachhani et al. (2006). In the work of Vachhani et al. (2006), labeled Unscented Recursive Nonlinear Dynamic Data Reconciliation (URNDDR), the prior was assumed to be a single Gaussian. In the proposed work, the prior is represented as a sum of Gaussians, which, in principle can approximate any arbitrary density function. Thus, the constrained updated sigma points represent the means of the updated individual Gaussians in sum of Gaussian density that represents the UGSF posterior. Another difference in our approach relative to URNDDR is the nonlinear update (in measurement) of the weights and update in covariances of the individual Gaussians used in the Gaussian Sum representation of UGSF posterior density. This, thus, results in a Constrained Unscented Gaussian Sum Filter. Simulations on benchmark case studies show that the proposed constrained UGSF significantly outperforms the URNDDR approach.

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Systematic Control Structure Evaluation of Two-Stage-Riser Fluidized Catalytic Pyrolysis Processes

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Commercial routes for propylene production are steam cracking of naphtha or liquid petroleum gas together with fluid catalytic cracking of heavy hydrocarbon liquids. The discovery of shale gas reserves around the world has driven the transformation of feedstock for steam cracking processes from naphtha to ethane. Compared with naphtha cracking processes, the propylene production of ethane cracking processes can be ignored. It can be therefore expected that the supply/demand gap of propylene will expand. Modifications on existing fluid catalytic cracking, compared with those various "on-purpose" propylene production approaches actually are more cost/energy-efficient routes to address the issue of propylene availability. Two-Stage-Riser Fluidized Catalytic Pyrolysis (TSRFCP) for maximizing propylene yield has been proven as an effective approach to not only enhace the propylene yield and feedstock utilization but also maintain the gasoline/diesel yield.1 In the TSRFCP process, fresh feedstock (raw oil) dispersed with steam is fed to the first-stage-riser and subjected to a certain degree of catalytic pyrolysis reactions. Dispersed with steam, the recycling oil from the downstream fractionator is introduced into the second-stage-riser and subjected to further pyrolysis reactions over the regenerated catalysts with good activity and selectivity up to the final conversion. Two risers share the same disengager and regenerator. Coked catalysts with low activity and selectivity are separated from the oil products at the end of each riser to suppress further thermal and catalytic pyrolysis. Oil products from these two risers are separated in the same fractionator. The regenerator is designed with a high-efficiency combustor and an external catalyst cooler.

Complex nonlinear behavior caused by strong interactions between exothermic reactions of catalyst regeneration and endothermic pyrolysis reactions along with stringent requirements on operations call for high-efficient control mechanism for the TSRFCP process. To some extent, the selection of the proper primary control structure is far more important than the detailed algorithm used in designing the actual controllers for a given structure. Based on the developed and validated mathematical model of an 12Kt/y demonstration TSRFCP plant, through the application of open-loop and closed-loop steady-state multiplicities, the primary goal of this article is to obtain the best control structure from candidates selected based on heuristic reasoning for a TSRFCP process which can maximize propylene yield without any significant losses in gasoline/diesel yields. Steady state multiplicity analysis can not only elucidate the relationships between potential manipulated variables and controlled variables over a large operational horizon but can also identify the perfect control action for tackling uncertainties in each control structure. It is illustrated that output temperatures from the two risers and the regenerator controlled by two regenerated catalyst flow rates and the cooling water flow rate, respectively, which have the best controllability characteristics and most superior dynamic behavior, are the most suitable control structure for further control system design of the studied process.

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[830]

Novel Data Segmentation Methods for Data Driven Process Analyses

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With the advent of computer control and Distributed Control System (DCS), process industries are storing a huge amount of data every day. These data are a rich source of information. Often time it requires selection a window of data from a large data set for calculating or estimating various performance metrics of the control loops or the process itself. For example, if data is collected at a sampling rate of 5s, there will be 17,280 samples for each variable every day. Calculation of a performance measure or metric requires only a few hundred or a couple of thousands of data points. The question is which part of the data should be used. This study attempts to find suitable data segmentation methods appropriate for the various purposes of data analysis. This study utilizes various simple statistical measures such as auto-correlation function, standard deviation and co-efficient of variation for selecting appropriate segment of the data. The performance of the segmentation methods is to be evaluated using simulation examples and real industrial data sets. The selection of appropriate window of data will largely increase the reliability of the data driven analyses.

[839]

Robust Model Predictive Control Strategy for LTV and LPV Systems of the Internal Reforming Solid Oxide Fuel cell

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Solid oxidefuel cell (SOFC) is an electrochemical device operating at a high temperature,converting the chemical energy of a fuel directly to electrical energy.Moreover, it can directly convert hydrocarbon fuels to a hydrogen-rich gas viainternal reforming inside the fuel cell stack itself. However, the endothermiccooling effect resulting from the reforming reaction at the anode side causesthe temperature gradient and thermal stress within the fuel cell stack. Thisrequires an efficient control design for assuring a stability of the system. Inthis study, a robust linear model predictive control (MPC) based on uncertainpolytopic approach is synthesized for controlling the SOFC. Different designsof the robust MPC using linear time-varying (LTV) and linear parameter varying(LPV) models are studied. The state feedback control laws are derived byminimizing a upper bound on the worst-case performance cost and are implementedto the cell voltage and temperature controls of the direct internal reforming SOFC.The simulation results show that under model uncertainties, the proposed robustMPC can control the SOFC when disturbances in the fuel feed and air temperatureare introduced and guarantee the stability of the SOFC. The performance of the MPCusing different linear models is compared and discussed.

[934]

Plantwide Predictive Monitoring of Sulfur Emissions in Tail Gas Treatment Units

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Plantwide predictive monitoring is a useful tool for observation of certain compounds of interest (e.g. pollutants) depending on fluctuations in the feed stream and operating conditions of plant sections. A general framework for the dynamic modeling of packed bed reactors (PBRs) in sulfur tail gas treatment is broached and implemented for related processes and a wide range of operating conditions. The model was validated using experimental data from both a miniplant for industrial off gas treatment and an industrial plant for sulfur recovery. After its validation, the model has been coupled with the existing multiscale models for thermal furnace already adopted to simulate Claus processes to get the plantwide prediction of plant emissions. The proposed approach allows to carry out a priori the estimation of environmental impact according to the current feedstock and operating conditions as well as to exploit in advance the hidden potential of the plant in mitigating/removing them before achieving the stack.

[949]

Robust control of industrial propylene-propane fractionation process

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Propylene is a raw material particularly important in the petrochemical and plastics industries. In this context, the control of propylene – propane mixture fractionating presents a great importance from the point of view of obtaining propylene specified purity (99.99%) and from the point of view of energy consumption. This paper aims to validate the dynamic simulation of robust quality control structures into industrial fractionating column of propylene-propane mixture.

The paper is structured in four parts. In the first part are analyzed following: multivariable nature of the process, quality specifications associated for separate products, energy issues and the types of control structures applicable to this process.

Second part of the paper analyzes the monovariable control structures for the separated products into industrial fractionating column. For the beginning, are identified the controlled variables and the available manipulated variables. Through use of Stationary Relative Gain Matrix (SRGM) were analyzed five possible structures for products quality control. SRGM components were computing through stationary simulation of the process, using Unisim Design® simulator. From the analyzed structures, the structures called L-V and L-B can be implemented in the industry.

The third part of the paper details the control structures selected by using SRGM. It highlights the theoretical and practical observations regarding industrial implementation of control structures.

The last part of the paper aims to validate the best quality control structure for separate products. For this aim is using Unisim Design® Dynamic Simulator. The fractionating column model was configured so that to reflect as real the behavior of control structures L-V and L-B. The utmost attention has been paid to the implementation of quality control systems and to the controllers' tuning. The simulation was intended to identify the behavior of structures L-V and L-B at modification of disturbances (flow rate and composition of feed flow) and references (the desired concentrations of propylene at the top and bottom of the column). The results of dynamic simulations demonstrated the superiority of the structure L - B.

[969]

Improved optimization-based design of PID controllers using analytical gradients

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The simple three parameter PID controller is the most adopted controller in the process industry. However, finding good parameter values by trial and error is not only difficult, but also time consuming. In combination with simple models, good parameters are usually found using tuning rules like Ziegler-Nichols or SIMC.

When the design complexity increases, in the form of process model complexity or special requirements on controller performance or robustness, it is beneficial to switch to optimization-based design. Here the requirements can naturally be translated into a control objective and constraints. However, this usually results in non-convex and non-linear problems, which can be hard to solve. This is especially true if the process has time delays.

The background for this study was to find optimal PID controller settings for a first-order plus delay process, and also to find optimal settings for a Smith Predictor controller. Here, the performance requirements were to minimize the integrated absolute error (IAE) for load disturbances and the robustness criterion was to have a given sensitivity peak (MS). To include the sensitivity peak specification, the frequency response was gridded.

When applying standard optimization methods using finite-differences to estimate the gradient of the cost function and constraints with respect to the tuning parameters, the optimization algorithm frequently fails to converge to the solution. Surprisingly, this also happens even though the initial point is very close to the local optimum. In our case, it seems that the main problem is not necessarily the non-convexity of the problem and the possibility for local minima, but rather inaccuracies in the estimation of the gradients when using finite-differences. We found that the robustness of the optimization was significantly improved by supplying the exact gradients.

In this paper we derive exact gradients for several performance and robustness specifications, including the IAE of the time response and the peak of the sensitivity function (MS). Deriving these gradients is not easy, but by masking use of certain properties of the system, we have derived analytical gradients for both Delayed State Space and Laplace models. The approach can also be easily extended to other performance and robustness objectives. The main advantage of using accurate gradients is that we improve the convergence properties and make the problem less sensitive to the initial point. We also obtain some reduction in the computation time (number of iterations)

The approach has been successfully used to derive optimal PID and Smith Predictor parameters for a large family of first-order with delay processes, and can easily be extended to other processes.

[973]

Enhancing xylitol bio-production by an optimal feeding policy during fed-batch operation

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The xylitol production has become an important process to investigate given the diverse product applications, especially in the food industry. The biotechnological xylitol production has been assessed mainly through an experimental approach via batch and fed-batch operation. This study presents an analysis for optimal operation of the fed batch process following a systematic methodology. The model based approach includes the collection, validation and calibration of the mathematical model, followed by the proposal of some operation scenarios. The implementation of such methodology allowed to increase 20% the yield of xylitol compared with the obtained previously in some experiments. Moreover, an analysis for the diauxic phenomenon was also performed, allowing to determine an optimal feeding ratio between substrates.

[981]

Performance Evaluation of Bayesian State Estimators for Nonlinear DAE Systems Using a Moderately High Dimensional Reactive Distillation Column Model

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Reactive Distillation (RD) systems can exhibit steady state input and output multiplicity behaviour due to complex interaction between reaction and phase equilibrium [1]. Occurrence of the multiplicity behaviour in the desired region of operation of RD systems poses challenges in monitoring and control of these systems. The difficulties are further compounded by the fact that dynamic models for RD systems often turn out to be a set of coupled stiff differential algebraic equations (DAEs). Occurrence of the output multiplicity behaviour leads to an open loop unstable dynamics at some of the multiple steady states. The behaviour of the process in the presence of output multiplicities, thus, depends on the process history and the process output can be different for the identical input moves. If it is desired to control the system at one of the unstable operating points, then use of a reliable nonlinear state estimator becomes an essential step in the controller synthesis. As a step towards observer based controller synthesis for a RD system exhibiting multiplicities, this work aims at carrying out a comparative evaluation of the performances of two recently developed nonlinear Bayesian estimators for systems modelled as DAEs, namely extended Kalman filter (EKF) and unscented Kalman filter (UKF) [2]. Efficacies of DAE-EKF and DAE-UKF have been evaluated by simulating state estimation problems associated with a benchmark ideal RD column [3], which exhibits input and output multiplicity behaviour simultaneously. In contrast to small dimensional examples considered in the available literature [2], the RD model considered in this work is of moderately high dimension i.e. it consists of 90 differential states and 21 algebraic states. The performances of the DAE observers are investigated in the neighbourhood of an unstable operating point of the RD system by assuming that only the temperatures on alternate trays are measured. Two performance indices, namely sum squared estimation errors (SSEE) and average computational time for one sampling instant, have been chosen for comparison of the performances of estimators. When compared on the basis of SSEE, the DAE-UKF was found to outperform the DAE-EKF. In fact, the DAE-UKF was found to work even with a large mismatch in the initial state, whereas the DAE-EKF performed satisfactorily only when initial estimation error was relatively small. However, under the identical simulation conditions, the average computation time needed for the DAE-EKF computations is significantly less (by factor of 60) than the average computation time needed for the DAE-UKF computations. Contrary to the claims in the literature regarding the drawbacks of EKF, the calculation of Jacobian for local linearization in the DAE-EKF formulation was found to be significantly faster than the multiple integrations needed in the DAE-UKF formulation for carrying out the prediction step. Moreover, the performance of DAE-EKF was found to improve if the top and the bottom concentration measurements are included in the estimation problem. Thus, DAE-EKF was found to be better suited for development of an observer based controller synthesis.

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[1035]

State Estimation in Fermentation of Lignocellulosic Ethanol. Focus on the Use of pH Measurements

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Monitoring of biochemical processes is essential for fault-diagnosis, control and optimisation. However, a number of factors have hindered the development of advanced monitoring techniques, especially in comparison with standard chemical processes. Lack of appropriate sensors and the high nonlinearity inherent to biochemical processes are some of the main obstacles mong these factors. In this context, the continuous discrete extended Kalman filter (CD-EKF) is an appropriate tool for state estimation in biochemical processes. The nonlinearity of the model can be efficiently tackled by the CD-EKF since the sensitivity of the dynamic model is updated at each sampling time via ODE integration. Commonly this step is consumes a non-negligible computation time. However, sampling time in biochemical processes is usually relatively slow (>1 min) and computation time is rarely an issue. Another consequence of the slow sampling is that the nonlinearity between samples may be significant; the performance of other EKF formulations using linear approximations for the forecasting step is then insufficient.

In this contribution, we apply the CD-EKF to monitor the production of ethanol by fermentation of glucose and xylose issued from lignocellulosic biomass. A generic model of ethanol fermentation by S. cerevisiae was developed, focusing on the effect of inhibitors in ethanol fermentation, as they determine to a large extent the yield of ethanol. Then, the CD-EKF was implemented for common measurement strategies e.g. online pH and level complemented with offline measurements at a longer sampling time. In this case, pH proved to be a key magnitude since it relates directly to the ethanol production and, at the same time, it greatly affects the yeast metabolism. Since it depends in a highly nonlinear way on the states, a linearised expression is updated at each time step. With this implementation, the CD-EKF was proven as an efficient way to monitor the process.

An immediate application of the CD-EKF is to optimise the pH and feed flow open loop trajectory. In effect, to foster the production of ethanol a trade-off exists related to the pH level. Increasing the pH greatly decreases the effect of weak acids that act as inhibitors, in particular above their pKa. On the other hand decreasing the pH reduces the need of base addition, and helps to operate in a region where the uptake of xylose is most favourable. We demonstrate how the CD-EKF is useful to update the estimation of the states all along the batch time. In combination with a trajectory optimisation solved by control vector parameterization (CVP), the economics of the process can be considerably improved.

Other perspectives of this work include the estimation of cell biomass and the early detection of contamination by other microorganisms, such as lactic acid bacteria which is a major obstacle for the cost efficient operation of the process.

[1051]

Deployment of Explicit MPC on Mini Fuel Cell Vehicle

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The Model Predictive Control (MPC) has become a standard advaned process control technology due to its inherant ability to handle process constraints. Unfortunately, implementation of MPC requires expensive online computations thus limits its applicabitiy to industrial systems only. The advent of the technology of explicit/multi-parametric MPC also known as "MPC-on-a-chip" has not only eliminated this limitation but also triggered significant advances in the area of control theory and its applications by employing it on inexpensive microcontroller hardware platform. Explicit MPC bypasses expensive online optimisation computations by simple and efficient function evaluations to obtain the optimal control inputs as explicit functions of the system states. The objective of this paper is to demonstrate hardware-in-the-loop implementation of explicit MPC on embedded microcontroller platform deployed onboard fuel cell powered vehicle.

Fuel cells are electrochemical devices that convert hydrogen or hydrogen rich fuel directly into electricity. Fuel cells are more efficient compared to other combustion based technologies and offer a wide range of tangible environmental, economic and operational benefits. The fast dynamics of fuel cells involves complex interaction of mass transport, energy transfer and electrochemical kinetics. Control is critical for the robust operation of the system—ultimately essential for maintaining uninterruptable power demand under load variations. Furthermore, fuel cell system integration to automotive powertrain brings additional challenges affecting durability and performance of the overall system. The majority of fuel cell system failures and forced outages (~90%) are due to lack of system integration. To overcome these challenges, this work presents a prototype fuel cell vehicle with step by step procedure to deploy explicit MPC on a fast 'mbed' platform based on high performance ARM® CortexTM M3 microcontroller. This prototype hardware is built using DC motor powertrain and 30 Watt air cooled polymer electrolyte membrane fuel cell. The proposed architecture efficiently controls vehicle speed under the uncertain operational scenarios. We demonstrate that the proposed embedded MPC-on-a-chip architecture is an ideal choice for fuel cell powered systems.

[1068]

Dynamic Simulation and Analysis of Slug Flow Impact on Offshore Natural Gas Processing: TEG Dehydration, Joule-Thomson Expansion and Membrane Separation

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On offshore platforms, natural gas must pass through a conditioning process, in order to achieve certain exportation specifications. Dehydration processes are used to prevent hydrate formation, which can obstruct and damage pipelines and equipment. For the hydrocarbon dew point control (HCDP), heavier hydrocarbons are removed from the gas to avoid condensation on duct lines and subsequent gas processing.

In Brazil, the huge pre-salt discoveries bring a new challenge to gas processing: the high carbon dioxide content. This component is an acid gas and in presence of water, it is highly corrosive. An addition, the CO2 content lowers the natural gas calorific value. Therefore, with the new Brazilian perspectives, carbon dioxide removal processes are of great relevance to attend gas specifications and assure secure operation and transportation. The membrane separation process is recommended for high CO2 contents and has other advantages, such as a low capital investment, easy installation and operation, and low weight and footprint, which is an important matter for offshore processing.

Offshore platforms are constantly susceptible to charge flow variations, such as the slug flow, which is an intermittent flow that may be very severe to the process. It can cause many problems throughout the production process: low gas or liquid flow periods, followed by others with extremely high values, emergency stops due to high liquid level in separators, inundations, equipment corrosion and damage, besides high maintenance costs. These problems bring environmental and economic losses to the oil and gas industry and can affect the process safety.

Dynamic simulation allows the analysis of the process behavior in presence of system perturbations. In natural gas processing, the study of transient behavior is notorious because oscillations such as the slug flow can be frequent and it is important to understand how the process responds to these. Dynamic simulation also enables elaboration of control strategies, commissioning of controllers, training for operators, support for safety studies, simulation of process emergency situations or start up and shutdown procedures, study of project changes and capacity increase, besides others.

This project proposes an offshore conditioning process for a natural gas stream with high CO2 content with the following operations: high-pressure triethylene glycol (TEG) absorption for dehydration, Joule-Thomson expansion for HCDP control and membrane separation for CO2 removal. The objective is to simulate and analyze the process dynamic behavior in presence of slug flow oscillations. The simulation software used is Aspen HYSYS (V8.4). However, it does not feature the membrane unit operation. Therefore, the project also develops a dynamic extension for the membrane separation using VB programming. The membrane extension behaves accordingly with the reality of the operation, with rapid dynamic responses to oscillations. It is considered that the study provides good estimates for the process transient responses, despite showing directionalities due to its nonlinearity. In general, the results point to good controllability and overall robustness of the process, considering the slug flow's severe oscillations.

[1080]

Dynamic Analysis of Offshore Natural Gas Processing with Sub-Sea Supersonic Separators

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In natural gas conditioning on offshore platforms, an important step consists of adjusting dew points of water and hydrocarbons in order to meet export requirements, preventing damage during transport and sale. The dehydration should be performed in order to reduce the probability of hydrates formation, which can damage equipment and pipelines. On the other hand, the removal of heavier hydrocarbon fractions of the gas (Natural Gas Liquids - NGL) helps to avoid condensation in duct lines. In addition, the NGL has high economic value in the petrochemical industry.

These two dew point adjustments can be carried out in only one unit operation. It is the supersonic separator (3S), which produces high gas velocity increases (Mach> 2), causing coolings in the order of -20 or -30 º C. This will lead to precipitation of ice and condensation of the condensable components, while conditioning both the gas dew points. The supersonic separator is a promising technology for sub-sea gas processing. Oil, gas and water can be separated in a sub-sea primary separator. The gas would then be conditioned in the 3S and compressed for transportation through gas pipelines, while oil and water would be pumped up through the risers for top-side processing. This would also be valuable to prevent the occurrence of slug flow, since there would not be any gas in the risers.

The objective of this project is propose an offshore natural gas processing plant with sub-sea supersonic separators, then simulate and analyze its dynamic behavior. The simulation software used is Aspentech HYSYS (V8.4). However, it does not feature the supersonic separator unit operation. Therefore, the project also develops a dynamic unit operation extension for the 3S, using VB programming. In dynamic mode, oscillations in the charge stream are simulated in order to allow the estimation of the process transient responses. This enables the evaluation of stability aspects and operational safety of this proposal, as well as access the design and tuning of systems and control loops.

[1147]

Semi-Global Stabilization of Polymerization Processes using Extended Washout Filter-Aided Controllwer

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This work presents a design framework to modify the bifurcation characteristics and stability of high-dimensional, nonlinear, polymerization processes within specified operating regions. Semi-global stabilizations are achieved and oscillatory process dynamics in the vicinity of Hopf bifurcation points (HBPs) are attenuated. By exploiting stability boundaries in process design, a new optimization algorithm is introduced to circumvent the limitations of traditional washout filter-aided controller for more practical applications. This controller is used to operate a high-dimensional, Nitroxide–Mediated, Radical Polymerization (NMRP) in a continuous-stirred-tank reactor (CSTR). The algorithm adjusts the eigenvalues of the model Jacobian matrix to relocate the HBPs. It is shown to permit flexible modifications of the bifurcation characteristics, providing acceptable performance for reference tracking and disturbance rejection, and guaranteeing stabilization of solution branches in specified regions.

Maria-Ona Bertran, Thomas Bisgaard and Rebecca Frauzem (Eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. 31 May - 4 June 2015, Copenhagen, Denmark

Track 6. Abnormal Events Management and Process Safety

[30]

Automata Based Test Plans for Fault Diagnosis in Batch Processes

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Hardware failures are inevitable but random events in the useful life of a batch chemical plant. If these incidences are not efficiently diagnosed, the consequences can be very serious and even catastrophic. Generally speaking, two remedial measures can be considered to enhance the diagnostic performance of any given process, i.e., adding online sensors and/or implementing test plans. Although the former option has already been discussed extensively in the literature, the latter was rarely explored in depth. To address this need, Kang and Chang (2014) proposed an effective procedure synthesis method by making use of the untimed automata. However, the failure-induced abnormal system behaviors cannot always be characterized adequately with their models due to the lack of time-tracking mechanisms. An improved synthesis strategy is therefore developed in the present work to construct the test plans with the timed automata. With this proposed strategy, it is necessary to perform three specific tasks in sequence, i.e., (1) All embedded components in the given process are first described with timed automata according to a set of systematic model-building rules; (2) All fault propagation scenarios and the corresponding observable event traces (OETs) are enumerated next on the bases of the above models; (3) The optimal test plan for every OET is then established by incorporating an additional "test" model with the component models. Extensive case studies have been carried out in this work to confirm the validity and effectiveness of the proposed approach.

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[178]

Modelling and Monitoring of Natural Gas Pipelines: New Method for Leak Detection and Localization Estimation

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Pipelines are one of the most economical transportation solutions for natural gas and crude oil. However, leakage of the transported material from pipelines can harm the environment and cause explosions. In this research, we show a new natural gas pipeline monitoring method for detecting a leakage. With measurements of pressure and flow rate, the algorithm identifies and locates, and isolates multiple leaks in a network of pipelines under different scenarios.

We start from a one dimensional, non-isothermal model of natural gas transport in a pipeline considering the effect of ground temperature, inlet temperature, leak, and compressibility factor change in the flow process [1]. The effects of thermal properties on the flow rate and leak detection are studied. For a single pipeline without consumer usage, a dual Unscented Kalman Filter estimation method was applied. With parallel parameter estimation, the effect of thermal properties was estimated.

For the scenario of a straight pipeline with consumer usage, an observer method is proposed for leak detection. From the nonlinear isothermal flow equations, a linear equation was approximated with respect to the relationship between consumer usage and flow rate measurement at the end points of the pipe, under fixed boundary conditions (the pressure at the pump stations). Due to the time delay of the flow process in the pipeline, a linear observer with multiple time delay scheme is applied [2]. Assuming that disturbances are temperature and pump station pressure variations (unknown inputs), a final input observer with multiple delays was designed through solving a Linear Matrix Inequality (LMI) equation. The LMI is associated with the stability criteria of the estimation error [3]. An H-infinity norm is introduced to minimize the effect of measurement noise on the estimation error.

Finally, a multiple leak identification method is proposed. Multiple leaks can be disguised by a single leak at different locations based on the measurement data of pressure and flow rate. Identification and isolation multiple leaks simultaneously, still remains a challenge [4]. In order to isolate multiple leaks, a bank of observers and a moving horizon estimator are developed. Combining all the methods above, a comprehensive leak detection and control methodology is proposed to solve the problem of pipeline networks.

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[234]

Estimation and Uncertainty Analysis of Flammability Properties of Chemicals using Group-Contribution Property Models

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Process safety studies and assessments rely on accurate property data. Flammability data like the upper flammability limit (UFL) play an important role in quantifying the risk of fire and explosion. If experimental values are not available for the safety analysis due to cost or time constraints, property prediction models like group contribution (GC) models can estimate flammability data. The estimation needs to be accurate, reliable and as less time consuming as possible. Outliers from the model set can strongly influence the parameter estimation, such that the property prediction can be inaccurate in the end. Therefore, it is necessary to identify possible outliers and remove them from the experimental data set. The outlier detection should be simple, following the structure of the model and mathematically strict.

In this research project flammability-related property data, like UFL, are estimated using the Marrero and Gani group contribution method (MG method). The method considers the group contribution in three levels: The contributions from a specific functional group (1st order parameters), from polyfunctional (2nd order parameters) as well as from structural groups (3rd order parameters). The latter two classes of GC factors provide additional structural information beside the functional group. The contributions of all three factors are then summed up. The method is simple and easy to apply. Taking into account higher order groups increases the accuracy. Furthermore, the application range is high due to the high number of considered functional and structural contributions.

In addition to the parameter estimation an outlier treatment methodology is suggested that identifies outliers based on the empirical cumulative distribution function (CDF). The empirical CDF tries to estimate the true underlying CDF and is not restricted by the assumption that residuals should follow a normal distribution. Hence, it has a wider application range.

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

1) Data. Experimental flammability data is used from AIChE DIPPR 801 Database.

2) Initialization and sequential parameter estimation. An approximation using linear algebra provides the first guess. Then the 1st, 2nd and 3rd order parameter estimations are performed separately.

3) Simultaneous parameter estimation. The result of the sequential estimation serves then as initial guess for the simultaneous parameter estimation algorithm.

4) Outlier treatment. Data points that are not reasonably likely expected to occur according to the empirical CDF can be considered as outliers.

5) Comparison. Outlier treatment based on empirical CDF is compared to treatments based on Cook's distance and normal CDF.

[361]

Dynamic artificial immune system with variable selection based on causal inference

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Large numbers of variables are measured in typical chemical processes. In most of the fault detection and diagnosis methods, all the measured variables are selected. However, the incorporating measured variables that do not provide any additional information about faults degrades monitoring performance, as Ghosh, Ramteke and Srinivasan illustrated in their work [1].

Artificial immune system (AIS) is a new artificial intelligence methodology shows strong ability of self-learning and self-adaptability. Much work has been done on its application in process monitoring and fault diagnosis in chemical processes. However, there is little research in the variable selection in AIS. In this paper, we propose an approach to optimize the variable selection for AIS. The approach is based on the causal inference among the measured variables. Through causal inference, the cause-effect relations among variables can be found and then variables that do not reflect the main trends of changes of the processes can be picked out. Then the variable selection of the AIS can be optimized and the performance of the fault detection and diagnosis of AIS can be improved. Case studies based on the Tennessee Eastman process and experimental distillation columns are performed to illustrate the effectiveness of our approach.

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[413]

A smart safety system for chemical processes

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Conventional safety systems are designed to mitigate incidents, i.e., they aim to reduce the impact of failures using relief valves, rupture disks and, usually, cause a system emergency shutdown. The design of these systems is based on failure likelihood and the accident severity. However, this basis is normally obtained empirically, leaving the safety system vulnerable to process nonlinearities. In addition, operating procedures are fulfilled with a lot of human interference. According to Venkatasubramanian et al. (2003), 70% of industrial accidents are caused by human errors. In this work, we propose a simulation-based approach considering several failure scenarios in a chemical reactor to determine the potential hazard to which the system is subjected. Depending on this potential, preventive actions can be taken in order to guarantee the reactor safety and integrity and to avoid a potential shutdown. These actions are calculated to provoke the least possible disturbance in order to reduce the impact on product quality, while keeping the process operating. The goal is to increase annual operating time of the plant without compromising the safety of the process and product quality. The simulation of failure scenarios is based on a first principles nonlinear model. Such approach increases the accuracy of the predictions and reduces the empirical nature of operational decisions. The behavior of the control system is also considered by using a nonlinear model predictive control (NMPC) and a moving horizon reconciliation technique to estimate the model states and parameters at each sampling time. When a simulation response indicates a hazard, the operating conditions are changed in order to accommodate a possible failure, guaranteeing that safety limits will not be violated and, simultaneously, disturbing the plant as less as possible, to reduce impacts on product quality. The estimation of the new setpoint is mathematically formulated as a multivariable optimization problem with constraints. The results show that the proposed approach is feasible for real-time applications and, providing a reliable model and an efficient fault detection system, unnecessary shutdowns can be avoided.

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[556]

Quantifying the electrical demand response capability of industrial plants by analysis of the safety and interlock systems

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Increasing electrification of the process industries, together with increased generation from variable renewable sources, is starting to cause concern about reliability of electricity supplies. An unplanned shut-down of an industrial plant may result from power imbalance caused by inadequate electricity supply leading to lost production, monetary losses, compromised mechanical integrity of process equipment, and safety concerns. A shut-down might, however, be avoided by temporarily changing the operating set-points of process units to reduce their power consumption in response to detection of a power imbalance. Such a response is referred to as variable operation.

Electrical demand side response schemes involving participation of industrial plants, in particular contingency reserve services involving load shedding, have recently been reviewed by [1]. In load shedding, all or part of the industrial load is disconnected to achieve power balancing. As an alternative to load shedding, the work proposes to assess the capability of an industrial plant to adopt variable operation.

Devising a variable operation strategy involves the quantification of set-point change limits. To do that, the continuous nature of industrial processes and the propagated effects of a set-point change through the process are considered. The aim is to quantify the plant-wide capability for variable operation by the analysis of limits on the safety and protection systems in the plant. Every unit is equipped with a safety and protection system which triggers tripping actions when the operating conditions deviate beyond the pre-set limits. A variable operation strategy must consider all process alarm limits to avoid unnecessary trips as the effects of a set-point change propagate through the process. The alarm limits are compared by expressing all the limits in terms of one useful quantity called the equivalent quantity. The equivalent quantity limits are calculated by means of process modelling, and then compared to find the most stringent limits. These critical limits characterise the overall capability of the plant.

The work will discuss the necessary specifications for a process simulator that will enable the analysis, and will give guidelines for deciding which is the most appropriate equivalent quantity to characterise variable operation in a particular situation. It presents a case study in a heavy oil processing facility in which a pump provides variable electrical operation by changing its speed set-point. The pump flow rate is chosen as the equivalent quantity. The low pressure alarm limit on a downstream heater is found to be the critical limit, which corresponds to 9% reduction in flow rate. Hence, the lowest allowable pump speed must be that which corresponds to a 9% flow rate reduction, to avoid tripping of the downstream heater, which would cascade into a plant-wide shut down.

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[662]

Evaluating Process Models for use in Construction of Safety-System Failure Probability Distributions

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Safety is a top priority for chemical manufacturing processes – accidents have the potential to be very costly, leading to loss-of-life or environmental catastrophes. Safety systems are designed to arrest abnormal events (i.e., disturbances control systems can't arrest). No safety system is perfect – every safety system has an associated failure probability. If the safety system failure probabilities were known by plant operators in real-time, informed decisions could be made to prevent processes from shutdowns or accidents. These probabilities can be difficult to estimate, and have gained significant attention from the research community. A popular choice for estimation has been through the use of dynamic risk analyses using Bayesian analysis. Prior distributions for safety-system failure probabilities are used in conjunction with likelihood distributions to form posterior distributions in real-time. Prior distributions are classically derived from expert knowledge, and likelihood distributions are data-driven. When data are sparse, often because safety systems are rarely activated, the prior distribution is weighted more heavily.

This paper focuses on techniques to improve the quality of prior distributions using dynamic process simulations to supplement sparse data. Many simulations of hypothesized, special-cause events are run, and meaningful statistics are derived to construct prior distributions. These dynamic simulations involve models of important process equipment, control systems, and safety systems. The quality of process model has a direct impact on the statistics. This paper introduces quantitative methodologies for evaluating models in risk analysis. High-fidelity models are computationally taxing, but provide more meaningful information for safety-system analyses. Conversely, while low-fidelity models solve more rapidly, they lead to more misleading results. Strategies for introducing parametric and nonparametric uncertainty are presented, leading to qualitative rules for model selection, as well as quantitative measures for improving risk analyses.

To demonstrate the effectiveness of these strategies, earlier work to create simulation models for steam-methane reformer (SMR) processes (Moskowitz et al., 2014) is extended.

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[691]

Risk Analysis Applied to Bioethanol Dehydration Processes: Azeotropic Distillation versus Extractive Distillation

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Azeotropic and extractive distillation systems are two options for the separation of azeotropic mixtures. In both cases, the use of a solvent, or entrainer, is needed to aid the separation task. Although the selection of solvents has been commonly based on their technical and economic implications, aspects such as safety are particularly relevant because they are closely tied to the physical and chemical properties of the solvent. Safety considerations are typically dealt with after the process has been designed; therefore, the effect of variables such as the use of a given solvent in separation systems is not considered during the design of the process. In this work, we describe a procedure to account for risk and safety, in addition to economic evaluations, as part of the process design. A probabilistic methodology is used, with the evaluation of a distance likely to cause death as a risk index. The safety assessment combines a frequency and consequence analysis to calculate risk. The approach is applied to the design of ethanol dehydration processes, for which azeotropic and extractive distillation systems are considered.

For the azeotropic distillation scheme, the use of n-octane as entrainer is assumed, while ethylene glycol is considered as the solvent for the extractive distillation process. The properties of the solvents affect the inherent process safety, since ethylene glycol is more toxic than n-octane, but less flammable. The comparison between the two alternatives is done in terms of individual risk and total annual cost. The procedure gives rise to a multi-objective optimization problem in which the minimization of such conflicting factors is carried out.

[744]

Shape Constrained Splines with Discontinuities for Anomaly Detection in a Batch Process

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A previously developed technique for qualitative trend analysis (QTA) based on shape constrained splines (SCS) has been favourably compared to pre-existing techniques for the purpose of batch process diagnosis. Thanks to the branch-and-bound algorithm, this approach leads to a deterministic and global solution for QTA. One limitation of this method is that local discontinuities in otherwise continuous derivatives of the fitted spline function are not permitted. Recent work however allows to relax the optimization problem further so that provable bounds can be computed for this more complicated case. In this contribution, the resulting shape constrained splines with discontinuities (SCSD) method is applied for anomaly detection in batch process data. Importantly, the QTA approach to anomaly detection proves worthwhile because (i) tuning of the SCSD method is limited to setting an upper control limit, (ii) the resulting sum of squared errors statistic shows almost no drift for SCSD in contrast to the similar Q-statistic computed by principal component analysis (PCA), and (iii) true positive rates by means of SCSD are over 80% while the PCA method delivers at most 70% for false positive rates up to 5% based on a data set consisting of 410 batches.

[774]

Quantifying Model Uncertainty in Scarce Data Regions – A Case Study of Particle Erosion in Pipelines

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The transport of solids in multiphase flows is common practice in energy industries because of the unavoidable extraction of solids from oil and gas bearing reservoirs. The safe and efficient operation and design of these pipelines requires reliable estimates of erosion rates. The models used to calculate this rate have significant uncertainty due to the complexity of the underlying process. This uncertainty becomes especially important during the design phase for subsea applications, as erosion rate allowance, which is set using the erosion rate predictions and its uncertainty, directly impacts the integrity of the facility. Unfortunately, none of the models provide an estimate of this uncertainty. This paper introduced a systematic approach to quantify the model uncertainty for erosion rate predictions combining Gaussian Process Modeling (GPM) with data transformation and cross-validation techniques. The results reveal that given the available experimental data and the erosion rate prediction model considered, the model uncertainty is on average 3.61 times the model's predictions. Hence, our results suggest at least on average four order of safety factor when designing subsea systems.

[961]

Leak Identication using Extended Kitanidis-Kalman Filter

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If it is desired to maintain uniform performance in the face of the soft faults, such as biases or drifts in system parameters or unmeasured disturbances, or hard faults, such as leaks in storage tanks, then it is important to diagnose them as they start developing and plan remedial measures. In particular, extended Kalman filter based fault detection and diagnosis approaches are of particular interest in this work. Wilsky and Jones [1] originally proposed a method for identifying time, location and magnitude of a fault using the generalized likelihood ratio (GLR) method. Deshpande et al. [2] have recently developed a nonlinear version of the GLR method. This approach is based on analysis of innovation or model residual sequence generated by the extended Kalman filter after occurrence of a fault. One difficulty with the GLR method is that it is necessary to assume a model, such as step or ramp function, for all anticipated faults while carrying out the diagnosis. Kitanidis [3] has proposed an alternate version of linear Kalman filter (referred to as Kitanidis-Kalman filter or KKF), which modifies the observer gain calculation step to make the estimated states insensitive to unknown input / faults of arbitrary character. Madapusi and Goyal [4] have recently used this approach to estimate magnitudes of the unknown inputs from the innovation sequence generated by the. The Kitanidis-Kalman filter, together with the input magnitude identification step, appears to be well suited for carrying out online fault isolation and identification. These developments, however, have been carried out for discrete time linear systems. Majority of the engineered systems, on the other hand, exhibit nonlinear dynamics in the desired range of operation. Thus, an extended version of Kitanidis-Kalman filter (EKKF), which can directly employ a nonlinear mechanistic model for fault / unknown input identification, has been proposed in this work. The proposed EKKF is then employed for isolation of faults, which can be modelled as drifts in model parameters. The residuals generated by EKKF are used to construct fault magnitude estimates. Thus, in addition to fault isolation, the proposed approach generates estimates of fault magnitudes for arbitrary variations in the fault. Efficacy of the proposed EKKF algorithm has been demonstrated using simulation studies on the benchmark quadruple tanks system [5]. Leaks occurring in the tanks are modelled as changes in area of the outlet for outflows from the tanks. The proposed EKKF based approach successfully identifies the leak type fault introduced in the tanks of the quadruple tank system.

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[1021]

Process Monitoring and Fault Detection in Non-Linear Chemical Process Based On Multi-Scale Kernel Fisher Discriminant Analysis

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This paper presents a multi-scale kernel Fisher discriminant analysis (MSKFDA) algorithm combining Fisher discriminant analysis (FDA) and its nonlinear kernel variation with the wavelet analysis. This approach is proposed for investigating the potential integration of wavelets and multi-scale methods with discriminant analysis in nonlinear chemical process monitoring and fault detection system. In this paper, a discrete wavelet transform (DWT) is applied to extract the dynamics of the process at different scales. The wavelet coefficients obtained during the analysis are used as input for the algorithm. By decomposing the process data into multiple scales, MSKFDA analyze the dynamical data at different scales and then restructure scales that contained important information by inverse discrete wavelet transform (IDWT). A monitoring statistic based on Hoteling's T2 statistics is used in process monitoring and fault detection. The Tennessee Eastman benchmark process is used to demonstrate the performance of the proposed approach in comparison with conventional statistical monitoring and fault detection methods. A comparison in terms of false alarm rate, missed alarm rate and detection delay, indicate that the proposed approach outperform the others and enhanced the capabilities of this approach for the diagnosis of industrial applications.

[1085]

Hierarchical Fault Propagation and Control Strategy from the Resilience Engineering Perspective: A Case Study with Petroleum Refining System

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Petroleum refining system is complex, non-linear, multivariate with a number of highly correlated process units. There exist strong nonlinear dynamic fault behaviors during fault propagation in petroleum refining system. In this paper, hierarchical fault propagation model (HFPM) is proposed as an extension of the Infrastructure Resilience-Oriented Modeling Language (IRML). The main contribution that consists in the design of HFPM is to incorporate the dynamic behavior of fault propagation. The model is divided into two parts. The first part is static analysis for system structure feature and the second part is dynamic analysis for fault evolution mechanism. The performance of the proposed model has been tested on atmospheric and vacuum distillation system. Based on the results illustrated in this paper, the proposed method can be used for fault propagation analysis in petroleum refining system and its modeling parameters can reflect structural feature and fault propagation behavior. Besides, HFPM can be further applied to the study on fault propagation trend prediction, fault tracing and resilience fault diagnosis in petroleum refining system.

Track 7. Plant Operations, Integration, Planning/Scheduling and Supply Chain

[69]

Supply chain design and planning accounting for the Triple Bottom Line

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The growing pressure from both costumers and governments towards sustainable development is redirecting strategies focused on profit to strategies that account for the triple bottom line, where profit, planet and people are considered. However, the complexity inherent to the integration of such decisions has been delaying the growth in both research and implementation of sustainable development practices. Therefore, decision support tools that adequately address such complex problems, both at a strategic and tactical level, should be developed to help companies adjusting to these current and growing sustainability pressures.

In this work, a multi-objective mixed integer linear programming (moMILP) model is presented for the design and planning of sustainable closed loop supply chains. It includes strategic decisions such as facility location, definition of the transportation network, technology selection and allocation, as well as tactical decisions such as supply planning, that satisfy the demand. The first objective accounts for the economical pillar of sustainability considering the profit maximization. The profit is measured through net present value (NPV) at the end of the planning horizon, accounting for costs with facilities, transportation, raw material acquisition, product recovery and human resources. The second objective is the environmental impact minimization, evaluating the environmental pillar of sustainability. It is measured using the Life Cycle Assessment (LCA) methodology ReCiPe, applied to the main activities of the supply chain: production, transportation and facility installation. Both unimodal and intermodal transportation are considered and their environmental impacts compared. The third objective accounting for the social pillar of sustainability is the social benefit maximization. This is measured through socio-economic indicators applied by the European Union to its Sustainable Development Strategy. An approximation of the Pareto front is accessed through the modified Ɛ-constraint method that allows to address the trade-offs inherent to these three conflicting objectives.

The applicability of the model is demonstrated through a representative supply chain case study showing how this tool may help companies to adjust to the new sustainability context.

[108]

Planning of a multiproduct pipeline integrating blending and distribution

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Pipeline scheduling is an important part of the petroleum supply chain. Pipelines have been used to connect refineries, harbors, depots, terminals and local marketstransporting crude oil and its derivative.This mode of transportation appears as the most reliable andpresents the lowest operational costto distribute large amounts of products over long distances. However, pipelines operation can be quite complex as it may involvenetwork pipelines, single or multiple origins and destinations, uni and bidirectional operations, pumping rates fluctuation and integration with upstream and downstream operations. Several researchers have proposed different models and techniques to solve the main features of pipeline scheduling problems but the problems of modelling multiproduct pipelines where input and output tank farms are considered simultaneously is still not enough studied.

On this context the present work addresses the scheduling for a distribution system characterized by a multiproduct pipeline that transfers a variety of products froma refinery storage tank farm to a distribution center. A discrete model formulation is developed to integrate pipeline scheduling with inventory managementat the refinery and distribution centers. Furthermore, it also considers that not all products at the product tank farm may be available to be transferredat any the time, so that the model becomes more realistic. The proposed approach takes into account daily demands, settling periods, forbidden products sequences and operating constraints aiming at the best pumping sequence and inventory profile while minimizing operational, pumping, inventorycosts. The developed Mixed Integer Linear Programming (MILP) formulation is applied to a real case-study and the results are evaluated in terms of quality solution,operational indicators, pipeline sequence and computational performance.

[113]

Optimal Multi-Period Investment Analysis for Flexible Pulp Mill Utility Systems

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The pulping process is typically continuous and designed for maximization of quality and throughput of one core product. The operational objective is to maintain the production as close to the design capacity as possible. Consequently, pulp mill energy systems are traditionally modelled using annual averages representing values close to design conditions. However, changes in wood, pulp and energy market conditions motivate a shift towards producing a larger variety of products including traditional pulp mill energy by-products such as electricity and heat, and emerging lignocellulosic biorefinery products such as different kinds of materials and chemicals. The transition from the traditional pulp mill towards a biorefinery concept will connect the pulp mills to an increased number of external markets. Also for the traditional by-products of heat and electricity, an increased implementation and production rate can be expected when energy prices rise. Pulp mills that are connected to district heating systems, which is common in Scandinavia today, can be strongly affected by large variations in heat demand over the day and over the year. In combination with the opportunities connected to the diversified product portfolio of a pulp mill biorefinery, there is no lack of incentives for better modelling of variations in investment analyses connected to pulp mill utility systems.

Methodologies for the design optimization of utility systems with varying demands need to simultaneously consider both design and operational decisions. Most published methods rely on a multi-period, mixed-integer linear programming (MILP) formulation. The present work suggests a multi-period approach for the specific application to a chemical pulp mill retrofit. The aim is to illustrate the potential advantage and importance of applying this kind of methodology also in an industrial sector such as the pulp and paper industry that traditionally has been served well by simpler approaches. In addition to boilers and turbine, the model proposed in this paper includes the option to invest in lignin separation, an emerging technology for the pulping industry. Previous work has shown that lignin extraction may provide a great opportunity for indirectly increasing the flexibility of the pulp mill utility production in response to demand variations. However, the previous study did not consider competing technologies, such as condensing power generation, which may have similar advantages. The aim of the present work is to extend the previous model with turbine models and investigate to what extent the lignin extraction can compete with the alternative of electricity generation. The model optimizes technology selection, equipment capacities and operating loads under the influence of demand variations, considering part-load efficiencies and operating load limits.

Application of the model to an illustrative example indicates an advantage for lignin extraction already at lignin prices above 22 €/MWh due to poor off-design performance of condensing power generation. This demonstrates the usefulness of the proposed modelling approach.

[114]

Scenario-Based Price Negotiations vs. Game Theory in the Optimization of Coordinated Supply Chains

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A scenario-based negotiation (SBN) win-to-win approach is proposed for the optimization of coordinated decentralized multi-site multi-product Supply Chains (SCs) in a competitive environment. Based on non-symmetric roles, the leader aims to settle its offer taking into account the uncertain reaction of the follower, which behavior is represented by a probability of acceptance. Different negotiation scenarios, based on considering Standalone, Cooperative, and Non-Cooperative SCs are analyzed for the negotiation, resulting in different MINLP tactical models, which are illustrated using a case study with different "follower" SCs around an industrial production SC "leader". On the other hand, a Stackelberg non-cooperative bi-level MINLP game model is built and solved for the same case study. The Non-Cooperative Negotiation Scenario (NCNS) proves to be more adequate, leading to higher individual profits expectations.

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[119]

On the complexity of production planning and scheduling in the pharmaceutical industry: the Delivery Trade-offs Matrix

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Traditional production planning and scheduling assume that product recipes and resource needs are known in advance and remain quite stable over time. However, the manufacturing of chemical-pharmaceutical products is preceded by complex development phases, where process design, planning, and scheduling problems are deeply related and that may not adequately be addressed in the existing literature. This work discusses the role of the production planning and scheduling of chemical-pharmaceutical manufacturing facilities. It starts by analyzing the main aspects that influence the planning and scheduling and proposes an extended scope of the related problems to account for higher levels of integration between process design and operational decisions. We argue that extending the traditional scope of planning and scheduling problems is particularly interesting when manufacturing products that are under development.

Following this argument we propose a novel conceptual representation, the Delivery Tradeoffs Matrix (DTM), to provide guidance on the tradeoffs occurring in the drug development process and to expose the factors that affect the performance of these manufacturing systems. The pharmaceutical industry recognizes the need for reducing time-to-market, the costs of new drug development, and the manufacturing costs. The path to efficient R&D and manufacturing activities will involve the introduction of new production technologies (Suresh & Basu, 2008), as well as, the adoption of innovative process design and planning and scheduling decision-making tools (Shah, 2004; Grossmann, 2012). The DTM depicts the current situation and a future situation as a possible response to the challenges the pharmaceutical industry is facing and needs to overcome. Through the proposed matrix, it is assessed the relative importance of: i) uncertainty and costs; ii) time-to-market and production volume; on the manufacturing activities involved in the development and delivery of the products. As a result, the presence of such aspects requires solving extensive problems that account simultaneously for design decisions. This will lead to an increase of the solution space of planning and scheduling decisions, thus clearly justify as target the global optimization of the operations.

[149]

Flare Minimization of Ethylene Plant Start-up via Resource-Task Network Approach

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Energy utilization andenvironment protection has received increasingattention over the last few decades. Therefore, flare minimizationhas become one of the main concerns for ethylene industry. Currently, the research of flare minimization has twomain approaches, which are the experience-based approach and the dynamicsimulation approach. In the experience-based approach, some improved methods havebeen presented to reduce flare emissions through experience andtrial. The most important improvement is starting charge gas compressors beforefeeding the furnace with start-up working medium, such asnitrogen, methane, mixed hydrocarbon, etc.However, theexperience-based approach has some limitations when it has to confront dynamic operations. In order to overcomethis shortcoming, Xu et al propose a methodology of flareminimization by using dynamic simulation tools, which includes three steps: steady-state simulation validation,dynamic simulation validation and dynamic simulation for start-up operation. However,the above method lacks optimization forthe start-up plans, which only adoptsdynamic simulation to validate the proposed startup plans. The start-up processof an ethylene plant can be considered as a semi-continuous process. Thus, theshort-term scheduling approach based on resource-task network (RTN) is firstly used in this paper to optimize the start-upplans.This work developed a flare minimization model for the start-up process of ethylene plant, whichcould overcome the aforementioned shortcoming. Theproposed model has been considered a universal method for ethylene plants tooptimize start-up plans. We analyzed the relationship between the key factors (thechoice of start-up working medium, the inventory of ethylene and propyleneproducts, and the utilities) and flare emission sources of start-up process. Accordingto the analysis, the RTN approach was used todepict the super-structure of the start-up process, in which the main featuresencountered in ethylene plant start-up process were definitely modeled. Then, we established the mathematical formulation of the flare minimizationmodel, in which a uniform type of time gird is used for allresources and tasks and eight types ofconstraints are involved to express the resource-task relationship. At last, the reliability and adaptability of the flareminimization model was validated by 5 significant casestudies. The results showed that the flare minimization model could effectivelyreduce the flare emissions and start-up durations.

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Phenomenological Decomposition Heuristic for Process Design Synthesis of Oil-Refinery Units

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The processing of a raw material is a phenomenon that varies its quantity and quality along a specific network and logics to transform it into final products. To capture the production framework in a mathematical programming model, a full space formulation integrating discrete design variables and quantity-quality relations gives rise to large scale non-convex mixed-integer nonlinear models, which are often difficult to solve. In order to overcome this problem, we propose the phenomenological decomposition heuristics to solve separately in a first stage the quantity and logic variables in a mixed-integer linear model, and in a second stage the quantity and quality variables in a nonlinear programming formulation. By considering different fuel demand scenarios, the problem become a two-stage stochastic programming model, where nonlinear models for each demand scenario are iteratively restricted by the process design results. Two examples demonstrate the tailor-made decomposition scheme to construct the complex oil-refinery process design in a quantitative manner.

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A Value Chain Optimisation Model for a Biorefinery with Feedstock and Product Choices

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There is a movement towards developing chemical sources from renewable or residual feedstock such as woody biomass or woodchips via biorefining. Value chain optimization is used as a decision making tool to aide in the development of biorefining.1 In this work, an optimisation model for the value chain assessment of a lignocellulosic biorefinery was developed using mixed integer linear programming. The model allows for the comparison of two different sources with different characteristics such as moisture content and size. Each source may be subjected to alternate pretreatment prior to biorefining to up to three product streams. Three versions of the model were developed: product-demand driven, biorefinery-capacity driven and supply driven. Optimization identified the most profitable locations for each process stage, including, collection points, pre-processing locations, biorefining locations and customers according to the associated transport, storage and processing costs. The case study was based around softwood in Scotland, UK, with two source streams, which were logged softwood versus the chipped by-product of the sawmill industry. Each source stream was subject to pretreatment to a certain moisture content and size, appropriate for the biorefining operation. The biorefinery was based on a technology developed by Bio-Sep Ltd which converts the lignocellulosic feedstock into three product streams, cellulose, hemicellulose and lignin. The results demonstrated the significant effect of moisture content on drying and transport costs, in addition to the preference of fewer pre-processing operations. Overall, it was demonstrated that decision making tools for biomass processing must allow for the consideration of these stages with respect to overall costs.

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Integrating natural hedging of exchange rate exposure in the optimal design of global supply chain networks

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Globalization of business is a major strategy of modern enterprises in order to comply with the shareholder wealth maximization principle. Seeking to explore sources of competitive advantage worldwide, enterprises expand their supplier base, their customer base, and their core operations into more and differentiated countries. Consequently, managing supply chains has become more complex and critical than ever before. Enterprises are struggling to design and operate more efficient supply chains capable of anticipating and addressing unknown and unpredictable risks inherent with their global presence.

One of the many risks that come with the global nature of supply chains is the risk of currency volatility. Foreign exchange rates can fluctuate dramatically over the course of a supply agreement and it is important to consider their impact upfront. To effectively manage long term exchange rate risks, enterprises should consider natural hedging strategies designed to manage risks through operational means. Natural hedging provides enterprises with flexibility in their supply chains by allowing dynamic adjustments in the locations used to manufacture, source, and sell. Such a flexibility enables to reduce the impact of large and long-term shifts in currency values on costs and revenues.

Although the issue of natural hedging in supply chains has challenged researchers (Ding, Dong, & Kouvelis, 2007; Kazaz, Dada, & Moskowitz, 2005), to the best of our knowledge a holistic multi-product and multi-echelon optimization model is lacking from extant literature. Our work aims to enrich the supply chain network (SCN) design literature by introducing a Mixed-Integer Programming (MIP) model that integrates natural hedging of exchange rate exposure with SCN design decisions. Typical SCN design decisions (facilities location, capabilities location, customer assignment, inventory management, distribution pattern, etc.) are accompanied with a set of natural hedging decisions (switching production locations, altering sourcing vendors, restructuring logistics network, relocating capacity, etc.). The proposed model is evaluated in terms of applicability and robustness in a real case study and the results are communicated with the readership. The model could assist and support managers in effective decision making for their global SCN's.

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[267]

Downstream Petroleum Supply Chains Planning under Uncertainty

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World economies have been struggling amidst financial crunches and soaring crude oil prices, which has increased the strain on the reduction of the petroleum products' retail price, in order for companies to stay competitive and sustain product sale volumes. The resulting market condition adjustments have created significant volatility among the petroleum prices, margins and product demand. As demand variations inversely follow price variations, the result is a constant need and consequently an opportunity for improving the efficiency of petroleum supply chains (PSC), namely downstream networks which must perform well in spite of price and demand uncertainty.

PSCs have always been under focus for supply chain optimization, specifically for refinery process design and scheduling. Lately, there has been an increase in the development of mathematical models for design, tactical and operational planning of upstream, midstream as well as downstream PSCs. Nevertheless, the integrated downstream PSC design and planning along with uncertainty management has seldom been targeted. As known, the PSC network design and planning problem spans many stages, entities, locations, transport modes, routes and products, hence is a large-scale problem. Additionally, uncertainty treatment renders them into stochastic NP hard problems.

Our recent research has focussed downstream PSCs for its collaborative design and tactical planning where the presence of collaboration amongst entities was found to be very positive for all entities. The current work departs from the previous work and develops an extended mixed integer linear program (MILP) to determine the design decisions relating to installation, sizing and operation of infra-structures, the fair price strategic cost and tariff decisions and finally tactical decision for periodic depot and route product affectations and inventory levels. The PSC network collaborative design and tactical planning is considered where simultaneous incorporation of he expected net present value (ENPV) maximization and reduction of risk considering risk measures is accounted, Risk measures as variance, variability index and conditional value-at-risk (CVaR) for multiple scenarios are explored, determining Pareto optimal solutions, thereby obtaining trade-offs. The model results are presented for different real case examples based on the Portuguese PSC network, which are compared providing insights and opportunities for further research.

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Optimal Management of Shuttle Robots in a Laboratory Automation System of a Cement Plant

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With the global trend in construction to use concrete instead of mortar, the product quality of the required cement plays an increasingly important role. To analyse the quality of the cement, small material samples are collected online in several steps of the continuous cement production process, and the composition of the raw materials and the additives in the samples is cyclically analysed. Based on these measurements, various control parameters are adjusted. In state-of-the-art cement plants, the sample collection, transportation and analysis is partially automated in a cooperative setup of a human-machine laboratory to minimize the time between the sample collection and the adjustment of the control parameters. It shows that rigorous optimization of the sample scheduling can lead to efficiency increases in an industrial real-world shuttle-based laboratory automation system that is connected to a cement production plant. In this system, the samples are collected and analysed in regular intervals and can be combined with additional samples that are started in collaboration with human workers with unknown arrival times. The human workers are able to directly access and use the analysers, making them unavailable for the automation system for a certain time. Other uncertainties that have to be considered in the scheduling are resource breakdowns in the analysers and delays in the operations. Following the approach in [1], all possible 340 samples routes of the sample scheduling problem are modelled in a generic fashion using the modular framework of timed automata (TA). The movements of the shuttle robot are modelled similar to the modelling procedure for sequence-dependent changeovers, see [2]. Based on the current set of collected samples and the current state of the system, e.g. the current location of the shuttle robot, a developed model builder automatically generates the corresponding TA model. To handle the different kinds of uncertainties in an efficient and robust fashion, the TA-based approach, which was originally developed for standard batch scheduling problems, is extended to a reactive scheduling approach that employs a cost-optimal reachability algorithm to compute optimal plans for the collections, transportation and analysis of the material samples. The reactive scheduling approach combines the working principle of a moving window approach in which schedules are computed one after the other for timely overlapping windows with an explicit event handling procedure to quickly cope with deviations in the schedule execution. We show that, compared to a typical priority-based dispatching rule, this approach can successfully handle the different uncertain events and can lead to significant throughput gains and meet all process-related time restrictions.

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[309]

A Novel Approach to Predict Violations and to Define the Reference Contaminant and Operation in Water Using Networks

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In recent years, the efficiency of water use has received special attention from researchers around the world. In the industrial sector, many works have been developed, and all of those seek a common purpose: to develop a practical and robust methodology to produce an optimal network, i.e. that one with the optimal configuration among operations which makes use of water, minimizing the consumption of fresh water and maximizing its reuse. Many of these works have faced common problems, mainly when considering large-scale case studies with a large number of operations and contaminants. To perform mass transfer calculations, it is necessary to choose a contaminant to be the reference for the others. The techniques previously used for this election have resulted in violations of the maximum concentration in the network synthesis. One such approach is the algorithmic methodology called Water Source Diagram (WSD), which emerged as a simple and robust strategy. However, there are still some gaps regarding the choice of a proper operation and reference contaminant. This work presents a new approach to the WSD, linked with a strategy to define which is the best contaminant and operation for be the references. To pursue that, it was necessary to use a new predictive algorithm and optimality conditions. The algorithm identifies possible violations in some contaminant concentration limits and in which operation the violation(s) exists. If no violations are predicted, the network is generated by the traditional WSD algorithm. Otherwise, if any violation is present, it is necessary to decompose a set of operations in different regions, called here "blocks". The optimality conditions and the new algorithm are then set for each decomposed block. For those blocks with no violation, the traditional DFA is used, but for the block(s), which present(s) any violation in the contaminants concentration limits, a Bound Contraction Global Optimization approach shall be employed, resulting in a water network without violations. All optimized blocks are integrated at the final analysis. The method was applied to real and large-scale examples in the literature and validated in a refining unit in Brazil. The results show the simplicity, effectiveness and yet robustness of the method, approaching the results obtained by several authors in the literature those made only use of mathematical programming.

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MDP formulation and solution algorithms for inventory management with multiple suppliers and supply and demand uncertainty

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Supply chain of a manufacturing system contains various functional activities including procurement of raw materials from suppliers. To determine the inputs into the production system, one needs to manage the inventories of raw materials considering demands of intermediate products. One of the most important issues for the inventory management is that various sources of supply and demand uncertainty should be considered for long-term operation. Many models exist for random demands while the case of supply uncertainty has been studied far less in the past, despite its significance. Also in general, these decisions cannot be made by intuition or heuristic approaches because multiple criteria for supplier selection tend to conflict with one another. Therefore, in this study, we apply a systematic approach to consider diverse (sometimes, conflicting) criteria for supplier selection and to incorporate possible realizations of uncertainty into the decision-making process at the same time. This multi-period decision problem is formulated as a Markov decision process (MDP) with two exogenous information variables: lead time (delayed time between order releases and arrival) and demand. Also, as an alternative to independent random demands, Markovian demands are considered to capture the time-correlations in randomly changing economic and market condition. Decision policies are obtained from solving the MDP problem through exact value iteration, or approximation approaches to overcome the 'curses of dimensionality.' We use an approximate value iteration method with a linear model, and compare the results with those from the exact value iteration algorithms and other heuristic policies for a simple benchmark problem.

[337]

Optimal design of closed-loop supply chain networks with multifunctional nodes

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It is well-known, that the high purpose of an organization or goods company is to maximize value creation over the entire life-cycle of a product considering both forward and reverse logistics. Effective management of reverse flows can reduce costs and enhance sales. Therefore, in order to ensure high profit margins, it is necessary for companies to maximize value over the entire life cycle. However, cost savings is not the only reason forcing companies to introduce a circular viewpoint to their SCN's operations. Environmental requirements, social responsibility, and governmental legislation are the main, and nowadays essential, pressures leading to the evolution of reverse flow and closed-loop SCN modeling.

There is a plethora of models found in literature the last decade aiming to optimize both forward and reverse supply chain network's operation and design. Some of the recent works are these of Salema et al. (2010) who presented a generic model for coping with the simultaneous design and planning of supply chains with reverse flows, of Cardoso et al. (2013) who developed a mixed integer linear programming for the design and planning model for closed-loop supply considering simultaneously all processes and uncertain product demand and of Ramezani et al. (2014) who addressed a multi-echelon and multi-period problem in a closed-loop SCN design under a fuzzy environment with intergrading activities considering the transportation option, the quality and hybrid processing facilities.

Our work, aims at enriching the literature on supply chain network (SCN) design by introducing a general mathematical programming framework that employs an innovative SCN composition coupled with forward and reverse logistics activities by introducing a generalized node with fourfold role. The generalized Production/Distribution/Recovery/Re-distribution (PDR) nodes will substitute the traditional plants and distribution centers at the forward flow and the traditional collection and re-distribution centers at the reverse flow of the materials.

The objective is to minimize the overall capital and operational cost and determine the optimal structure of the network. The model defines: (i) suppliers; (ii) generalized node's location and role; (iii) material flow among SCN's levels; and (iv) functional elements (capacity, material flow, inventories, purchases etc.). The applicability of the SCN design and operation model is illustrated by using a representative supply chain case study.

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[342]

Simultaneous Optimisation of Economic and Environmental Objectives with Dynamic Price Signals and Operational Constraints

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Processing plants are often required to be capable of turndown or increased production depending on the demand for their products or changes to the raw materials supply and the design of the process should take into account these considerations in determining additional capital that may be required to provide this additional flexibility. In this paper the economic and environmental performance of a natural gas combined cycle (NGCC) power plant fitted with carbon capture and storage facility (CCS) is optimised under a number of different scenarios using a time-integration multi-objective optimisation (MOO) framework.

In the base case scenario, the plant is operated in a base-load continuous mode and just accepts the electricity price available. The economic performance of the plant will be modelled through the selection of four representative days (one for each season) and the hourly electricity price will be accepted for the 24 hour period on each of these days. The results are provided on a Pareto front multi-objective basis as annual net operating profit plotted against the average fraction of CO2 captured. This parameter is varied from 50% to 95%.

In the alternative scenarios, a time slice pseudo-steady-state modelling approach is used to integrate the performance of the plant over each of the four selected days. In option one, the MOO solver will maximise the profit and fraction of CO2 captured by allowing the operation of the capture plant to vary each hour with no operational restrictions on either it or the NGCC steam rankine cycle. The process parameters that may be varied include the capture plant solvent flowrate, stripper pressure and reboiler duty. Pareto plots for each decision variable are provided to show the extreme variations possible.

Option two recognises that there are restrictions to the maximum turn down that can be achieved on specific equipment, for example the maximum turn down on the solvent flowrate to the CO2 absorber is 60%, and with similar limits set for the steam system and the CO2 compressor. Under this option, a more restricted MOO is conducted and results presented.

Under both options one and two, the capture rate is reduced in order to allow for the production of electricity to be maximised. However, there is an additional dynamic that can be included in the analysis and this is the storage of CO2-rich solvent. Under options 3 and 4 scenarios, storage of both rich and lean solvent is permitted to allow CO2 to be captured during periods of high demand, but processed when the electricity price is low. Option 3 has unrestricted turn down, whereas option 4 has these constraints imposed.

By providing the results on an annualised basis for both operating profit and CO2 captured, the marginal cost of CO2 being captured can be obtained directly from the slope of each Pareto curve. The cost of the operational constraints as well as the storage facility is also directly obtained from the dynamic MOO analysis. This general modelling framework can be applied to a wide range of industries where there are similar economic and/or environmental dynamics.

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Operational scheduling of large industrial plant considering an electricity Demand Response scheme

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In the recent years, there has been a significant interest in improving the operation of energy-intensive industrial plants such as metals, pulp and paper and air separation (Merket et al. 2014). The scheduling of the operation of a plant provides a better coordination of the production and the maintenance tasks. The outcome of the scheduling is an increase of the efficiency, reduction of the total costs, such as maintenance and energy costs, and an increase of the life time of the assets of the plant.

Incorporation of energy management into the scheduling of the operation is a new topic which has to be investigated. The reasons for exploring the integration between production and energy management are that renewable energy sources are continuously taking a larger share in electricity generation (Merkert et al., 2014) and the global energy consumption is expected to grow in the next years. Renewable energy sources cause operational difficulties in the power system due to their unpredictable availability (for example wind availability). Large industrial consumers can help the power transmission operator to balance the power grid by participating in Demand Response schemes: for example, the industrial plants are required to reduce power consumption at peak times (dispatchable programs).

Mitra et al. (2012) presented a study on optimal production planning considering a non-dispatchable program, i.e. variable electricity prices, including a case study of an air separation plant. That work shows there is academic interest in examining the potential for industrial sites to participate in Demand Response schemes. The current study now considers the potential for a large plant like an air separation plant to become involved in a dispatchable Demand Response scheme.

The current study investigates the benefits and challenges of the integration between the optimization and automation system of an air separation plant and the dispatchable Demand Response scheme. It presents the problem in an optimization framework where the objective is to minimize the total costs of the air separation plant focusing on its air compressor station, which is the major energy consumer. The optimization suggests for example how much to load the online compressors and how much product to store in the buffer tanks considering the orders to adjust the consumption dispatched from the transmission operator. The results show how a large energy consumer can assess its ability to offer power reserves and how the trading of these power reserves might be quantified.

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[375]

Integration of Scheduling and Vessel Routing in Pipeless Plants

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Pipeless plants offer an alternative flexible production route to traditional batch plants, where different transferable vessels keep moving between stationary processing stations for performing typical operations such as charging, mixing, heating, cooling, discharging, and cleaning. The vessels are carried on automated guided vehicles (AGVs) between processing stations. Unlike in traditional batch plants, cleaning between product changeovers in the same vessel can be done at another cleaning station without losing production time. In the operation of pipeless plants, decisions have to be made regarding scheduling of production processes, assignment of orders to stations and vessels, and routing of the AGVs. The efficiency of operation of pipeless plants depends on the optimality of the production schedules. The optimal routing of AGVs must be determined for a safe and collision-free operation of transporting vessels from one station to another. Vessels are used for both processing and storage of materials in addition to transporting the batches from one station to another. Owing to this strongly interacting nature of the scheduling and vessel routing aspects for pipeless plants, they need to be addressed simultaneously using an integrating approach.

In this work, we propose an integrated model for scheduling and routing of vessels for a given layout of processing stations using state-task-network (STN) process representation and unit-specific event-based continuous-time formulation. In the development of STN, vessels are treated as separate states and the relevant tasks are converted into as many tasks as the number of vessels when the number of vessels available is less than the number of batches of all products to be produced. Otherwise, when there are more vessels available, then vessels need not be considered in states and tasks. The methodology used here involves addition of vessel routing tasks and routes as units. Herring-bone layout is assumed for processing stations. The different possibilities of feasible routes for different production sequences are considered as separate units. The travel of an empty vessel or a vessel carrying material on a route is considered to be a routing task. These routing tasks are product specific in order to maintain the identity of the production sequence. If a routing task repeats for a particular production sequence, it is considered to be different as it involves production and consumption of a different pair of states of material. The proposed methodology is demonstrated on an example from literature involving a pipeless plant producing three identical products with same processing sequence for each product using a maximum of three identical vessels available. There are seven stages of processing and eight units are available for production arranged in a herring-bone layout. The computational results were obtained for different number of vessels considered. The complexity of the integrated model was observed to increase with decrease in the number of vessels available.

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A Mean Value Cross Decomposition Strategy for Demand-side Management of a Pulping Process

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As energy is becoming a critical resource, it is important to include more energy awareness to industry's daily operations planning to reduce the total operating cost. The traditional approach is to schedule the production first, and from the schedule to predict the demand for energy [1, 2]. Then, energy purchase optimization models find the best available energy portfolio. This is not necessarily a system-optimal solution. Most reported methods in the scientific literature combine total scheduling problem with all energy-related information into a single monolithic problem. This ensures finding the system-optimal solution. However, it requires noticeable efforts to integrate both scheduling and energy planning into one model, and solve it effectively.

We propose a novel approach. We find that in some conditions it is possible to use the mean value cross decomposition strategy [3] for solving the total problem as separated models, the energy-aware production scheduling problem and energy-cost optimization problem. We find that the two optimizers can be modified such that they are a part of the sub-problem of the Benders' decomposition (energy-cost optimizer) and a part of the sub-problem of the Dantzig-Wolfe's decomposition (energy-aware scheduler). The models exchange two signals: dual information of the complicating constraint from the energy-cost optimizer, and the production scheduler's load curve.

We apply the developed method to a Thermo-Mechanical Pulping process using discrete-time Resource-Task Network approach [1]. The scheduling model comprises the minimization of deviation penalties as a result of committed load problem. In energy cost optimization we use the generalized minimum cost flow network model [2] to find the optimal structure of multiple time-sensitive electricity contracts including base load, time-of-use, day-ahead spot market and onsite power generation, and opportunity to sale electricity back to the grid with revenues. Both models are formulated using Mixed Integer Linear Programming (MILP) modelling and solved using realistic data instances. The results show that for practical industrial use cases the approach allows using existing models and obtaining very good quality solutions.

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[442]

Time representations for integrated batch process scheduling and water-allocation network design: A comparative study

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In the last 10 years, simultaneous optimization of batch process schedules and water-allocation network has received considerable research interest as a challenging problem in the process synthesis area. Batch water-allocation network (WAN) are time dependent, not only with respect to the water usage and wastewater generation, but also to the network architecture. This underlines the importance of process scheduling in the optimization of batch WAN. One of the key issues concerning process scheduling models is the time representation. Features and performance of different time representations for short-term process scheduling problems have been illustrated by Floudas [1].However, for an integrated batch process, the interactive relationship between production tasks and water-allocation tasks in time dimension will bring a whole new level of complexity to superstructure and models, which means new challenge for time representation.

Numerous formulations based on different improved time representations have been proposed in the literature. Three representative time representations are discussed in this paper: global event [2-3], global event and discrete time [4], unit-specific event and discrete time [5]. We will compare and evaluate the performance of four such models based on our implementations using two kinds of benchmark example problems from the literature: washing process-only and production-based water using process. Two different objective functions, minimization of effluent and maximization of profit, are considered, and the models are assessed with respect to different metrics such as the problem size (in terms of the number of binary variables, continuous variables, and constraints), computational times (on the same computer), and the quality of solutions. The effects of operation schemes, fixed and variable processing time, on the models are also considered and discussed. The insight comes from this comparative research will enhance our understanding on the role and the nature of time representation in the integrated batch processes and indicate the new directions to improve the models.

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Optimization of petrochemical process planning using naphtha price forecast and process modeling

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Naphtha is the first petroleum product during the distillation of crude oil and subsequently upgraded to make the major components of gasoline. Naphtha price forecasting is very important due to high price volatility. This has a global effect in its supply, demand, political situation of the world and weather etc. These considerations led to the optimization of petrochemical process planning considering naphtha price forecast and process modeling. This study was considered to analyze not only real forty five time series data of each factor but also qualitative factors. The data was normalized from 0 to 1. First of all, naphtha price was predicted using various methods such as multiple regression, exponential smoothing, Artificial Neural Network(ANN) and System Dynamics(AD) models. In order to validate the proposed models, the predicted naphtha price variations were compared with the actual naphtha price data. Secondly, petrochemical process was divided into cracking and reforming andd simulated considering chemical reactions involved. Process simulation was validated using reference plant data. Finally, petrochemical planning was optimized with naphtha price forecasting and petrochemical process simulation. This study is useful to decision-makers for petrochemical industry planning.

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Tighter integration of maintenance and production in short-term scheduling of multipurpose process plants

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In the continuous attempt to improve the performance of a manufacturing plant, production and maintenance scheduling play a fundamental role. A proper production schedule ensures the optimal usage of the plant by finding the best allocation of products to equipment and maximizes e.g. the production throughput and revenue. Maintenance scheduling is responsible for timely execution of maintenance activities on plant equipment (e.g. cleaning, parts substitution…) ensuring assets availability when needed by the production and possibly improving production quality and/or equipment performance. The interdependency between the two decision processes is frequently overlooked in literature and industry. Several contributions tend to limit the impact of maintenance on the production to a reduction of available equipment uptime. This is for example the case of the production scheduling approaches with equipment availability constraints, i.e. predefined time windows in which the equipment is not available for the production due to a prescheduled maintenance (Shah et al., 1993). In other cases, a set of maintenance requirements (i.e. equipment to be maintained, maintenance duration, time windows for the execution…) to be performed within the scheduling horizon is provided along with the production (Dedopoulos and Shah, 1995 and Hazaras et al., 2012) and a maintenance task is simply reduced to an additional job with special constraints to be scheduled on the plant. While the impact of maintenance on the scheduling of the production have been extensively studied (e.g. in term of equipment availability), the effect of the production on maintenance requirement has been highly underestimated. In this work, we propose an optimization based approach which tries to close this loop. We consider a generic batch processing plant using a state-task-network (STN) representation of production recipes (Shah et al., 1993). Along with the standard production scheduling constraints (e.g. assignment of products to units, timing of operations…) we assume that each unit can work for a limited amount of time (RUL – Residual Useful Life) before requiring a maintenance operation which reset its life to as-good-as-new and imply some operational costs. We also assume that each production task performed by the unit "consumes" a part of its residual life time. We furthermore assume that any unit can work in different operating modes and that the processing time of a task on the unit as well as the impact of the task on the RUL of the unit are a function of the operating mode. An MILP formulation for the joint maintenance and production scheduling problem will be presented as well as computational results of the proposed approach on different production processes.

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[481]

Integrating Control and Scheduling based on Real-Time Detection of Divergence

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Scheduling and control have been long recognized as the two critical building blocks in many manufacturing execution systems. Operating at the interface between the supply chain and the process, the scheduler generates a detailed schedule that has to be executed by the process so as to meet the demands originating from the supply chain. The controller in turn seeks to ensure that the process is operated as per the set points specified by the schedule while rejecting disturbances. In a broader sense, both seek to insulate the system from undesired disturbances, while adapting to real-time changes in the operating environment (e.g.: sudden changes in demands, equipment availability, etc.) and simultaneously accounting for inertia in various forms (e.g.: inventory, resource availability, committed actions). Given the strong similarities and the tight interactions between the two, there has been wide interest in integrating control and scheduling [1-3].

A variety of methods ranging from monolithic integration into one large integrated problem, to hierarchical cooperative approaches have been proposed in literature. In this paper, we propose an alternate approach to the integration problem.

Our key insight is that disturbances which occur post the generation of the original schedule, trigger a divergence between operational targets defined by the schedule and its execution [4]. If left uncorrected, the disturbances will propagate between the process and the supply chain. A timely response could eliminate or minimize such effects. Recognizing this, we propose a novel framework for integrating scheduling and control that detects in real-time when a divergence occurs between the original schedule and its execution in the process, identifies the root-cause(s) of the divergence (i.e. the disturbance), and triggers a suitable response from the scheduler and the process so as to nullify or minimize its effect. In this paper, we will describe the proposed approach and illustrate it using an industrially motivated case study.

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Resource efficiency indicators for real-time monitoring and optimization of large integrated chemical production plants

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Increasing raw material and energy cost as well as the growing awareness of the environmental impact of chemical production processes call for the systematic monitoring and optimization of the resource efficiency. The environmental impact of the production is assessed by many companies, but only computed on long time scales, usually for a business year. Process operations have a significant influence but this influence usually is not transparent to managers and operators. The EU-project MORE [www.more-nmp.eu] is currently developing real-time resource efficiency indicators (RTREI) that can be used to steer plant operations towards improved energy and resource efficiency.

This contribution presents the principles of RTREI, which capture the current technical and operational performance of a given process on shorter time scales. This is done in order to provide assistance to managers and operators on how to improve the operation with regard to resource efficiency and economic performance.

Following a gate-to-gate approach, an integrated mass and energy flow analysis is conducted to evaluate all the significant streams that are crossing the system boundaries. Subsequently, specific REI (based on raw material, production, etc.) are derived which characterize the current process operation. These REI can be referenced against a best case value, either derived from historical data or from a model based theoretical analysis, which considers factors that cannot be influenced by operational decisions, such as ambient temperature or raw material quality.

Standard indicators are often not capable of indicating the total efficiency if an energy mixture of different sources is consumed by the process or certain streams are used both as raw materials and as carriers of energy. In this situation, a combined energy and material flow analysis is needed to indicate the true performance, especially in cases where a significant amount of energy is discharged or consumed by a chemical reaction.

To demonstrate the methodology, indicators for an ethylene oxide production unit operated at INEOS in Cologne are developed and compared to currently used KPI, proving the suitability of the proposed approach in industrial applications. The resulting REI are evaluated using the MORE-RACER evaluation process to identify which indicators are capable of reflecting the total resource efficiency best in real-time. The framework is based on RACER criteria ([1]) for the evaluation of retrospective key performance indicators and relies on a scoring scheme adopted from [2]. It is specifically tailored to the requirements for real-time indicators.

The methodology is applicable to a broad variety of sectors ranging from the health care industry over pulp and paper to refineries.

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A meta-multiparametric framework: Application to the operation of bio-based energy supply chains

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The limited availabity of fossil fuels and the concern related to the environmental impact associated to the use of this non-renewable resource have motivated the interest in the use of alternative technologies and biofuels for energy generation. One important practice is the use and exploitation of agroindustrial wastes (i.e. biomass) as a fuel (solid or treated) for several power generation systems with the main purpose of locally energy distribution so as to reduce energy losses and improve the responsiveness to energy demand fluctuations. The management of these situations generally faces to a challenging design and planning optimization problem which involves the capacities, cost and productions of the available energy generation units at each time instant. Additionally, the network management is directly affected by several types of uncertainty in which we can highlight the demand uncertainty. Therefore, in order to ensure the reliability of the system, uncertainty must be considered due to the fact that the deterministic solution may become suboptimal or even infeasible.

This paper proposes a framework for the analysis of complex optimization problems under uncertainty. The usual multiparametric programing approach is skipped through the use of metamodels to mimic a set of already solved scenarios. Such framework has been applied to the operation of a bio-based energy supply chain, taking into account economic, environmental and social aspects: these objectives might be summarized in a single-objective formulation according to arbitrary economic criteria so, in order to assess the importance of the weighting factors used in the final decisions at different demand levels, a Kriging based metamodeling technique has been used to simplify the optimization procedures, leading to dramatic reductions in both the complexity of the methodology application and the required computational effort.

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[633]

A Continuous-time MILP Model for Direct Heat Integration in Batch Plants

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Important constraints to be handled by scheduling models are those related to energy use. One active research topic concerns the incorporation of hourly changing electricity prices from the day-ahead energy market, so as to drive energy consumption from periods of high to low demand. In the proposed models, it is most of the time assumed that there is unlimited amount of energy available. This is no longer the case when dealing with heat integration in batch plants, where heat sources and sinks need to be synchronized for direct integration to happen. Even if a hot and cold stream overlap in time, the temperature of the hot stream is higher than the cold stream and the same heat is involved, the heat/cooling rate resulting from the integration for one of the streams (in K/h) may be too fast or too slow to be viable.

In this work, we deal with direct heat integration in a single stage multiproduct batch plant so as to minimize the total consumption of heating and cooling utilities. The industrial case study is the neutralization section of a vegetable oil refinery, where each product needs first to be heated and then cooled. A continuous-time Generalized Disjunctive Programming (GDP) formulation is proposed that considers the four possible alternatives of integration between a hot and a cold stream. It should be highlighted that a hot/cold stream may change heat with multiple cold/hot streams as long it happens in parallel. This assumption is based on the isothermal mixing assumption in the simultaneous approach for heat exchanger networks of Yee et al. (1990), which avoids the need for information of flows thus keeping the model as a MILP. In other words, a two-stage temperature location superstructure is assumed for each stream with one stage comprising the eventual heat integration and the other the utility requirement. The decision of whether the heat integration precedes utility usage is going to be determined by the optimization.

The developed GDP formulation is going to be reformulated into big-M and convex-hull MILPs so as to determine the most efficient model. Extensive tests will also be performed to determine the maximum size of the problem (in terms of hot and cold streams) that can be tackled in reasonable time.

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[642]

Optimal Scheduling of Liquid Drug Product Manufacturing

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The increasingly competitive pharmaceutical industry calls for advanced scheduling models, tailored to the specifics of drug product manufacturing. Optimized schedules support reducing required format changes and isolator sterilizations by optimal sequencing. In real-life, such schedules can only be performed reasonably by fulfilling all major production constraints in one model simultaneously, including demand, shelf-life, due date, workforce availability as well as capacity of utilities and equipment. On top of these constraints, redefining an optimal batch size and rescheduling of batches are frequent issues caused by reprioritization of products, raw material scarcity and sterile holding time limitations. Hence, optimal scheduling on the shop floor level is a very complex situation, which is paramount for increasing production efficiency.

In this work, most of the aforementioned challenges have been solved and a slot-based formulation is presented that was inspired by a liquid vial production line. While considering demand, shelf-life, due date, product-dependent processing rates and sterile holding times, the formulation allows finding the optimal batch order with respect to make-span minimization. This goal is achieved by the introduction of two operation modes, similar to the concept described by Mendez et al. (2014). The model includes batches produced individually, and the more time-efficient variant, where multiple batches are produced within a campaign, i.e., cleaning and sterilization activities are reduced. A second key feature of this model is the complexity reduction of the filling processes for liquid products. Such fillings are performed in several hundred working steps; however, grouping the filling tasks into process elements that need to be performed without major interruptions, e.g., weekends, allowed an efficient modelling with only ten process elements.

The formulation will be expanded to account for two parallel filling units and subsequent quality assurance steps, including a thorough visual inspection of product quality, laboratory testing and quality management release.

A case study considering a Parenterals manufacturing facility of Roche in Switzerland was used to validate and optimize a three-months production schedule; including orders of twelve biopharmaceutical drug products and respecting phases of technical services as well as media-fills. The difference between the make span for batches as scheduled for Q4 2014 by company experts and the schedule provided by the optimisation algorithm is over 2 % of the planning horizon, which entails important benefits to the process plant.

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[644]

Improving Pharmaceutical Batch Production Processes with Data-Based Tiered Approach

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Improving the yield of batch-wise production is an increasingly important topic for the pharmaceutical industry; reasons for that include the rising public pressure on drug prices as well as a number of soon-expiring patents. This study defines a data-based, three-level approach for yield enhancements in batch-wise operations that is applied exemplary to the manufacturing of sterile drug products. The application on data of a yearly Parenterals production validated the presented approach by facilitating the identification of the main loss causes (e.g., quality control samples and scratched vials) and by supporting the development of improvements with the result of an increased production yield. As a case study, one loss cause (i.e., rubber stoppers with embedded particles) is discussed, where all three levels were applied and a process enhancement could be realised.

[714]

Integrated Cyclic Scheduling and Operation Optimization for Cracking Furnaces System Considering Feed Changeover

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In the traditional scheduling of cracking furnaces group, the product yield is supposed to be only an exponential function of time with constant operation conditions, and feed changeover without decoking is not permitted. However, due to changeable market price and flexible feed resources, the feed changeover for cracking furnace occurs frequently. Meanwhile, flexible operation of cracking furnace gradually promotes, such as the advanced control, cracking severity optimization. The integration of scheduling and operation optimization is a promising way to further improve the performance of cracking furnaces group. Motivated by above situations, a novel integrated cyclic scheduling and operation optimization for cracking furnaces group considering feed changeover is proposed to meet this challenge. In this work, the dynamic model of ethylene cracking furnace is developed based on a commercial ethylene cracking furnace simulator Coilsim1D. The dynamic model is expressed by a surrogate model incorporating the state space model and feed-forward neural network. In the dynamic model, the coking rate, product yields and tube maximum temperature are corresponding with the time variable variables such as feed rate and coil outlet temperature. Thus, the integrated cyclic scheduling and operation optimization model is a mixed-integer dynamic optimization (MIDO) problem. Discretized by the orthogonal collocation on finite elements, the MIDO problem is converted into a large scale MINLP problem. A case study is used to demonstrate the efficacy of the developed integrated model.

[795]

MINLP Model and two-level Algorithm for the Simultaneous Synthesis of Heat Exchanger Networks and Utility Systems

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This work proposes a novel approach for the simultaneous synthesis of Heat Exchanger Networks (HEN) and Utility Systems of chemical processes and energy systems. Given a set of hot and cold process streams with given mass flow rates, inlet and outlet temperatures, and a set of available utility systems (e.g., cooling water, boiler, multiple-level steam cycle, refrigeration cycle, heat pump, etc), the method simultaneously determines the optimal selection of utility systems, their design, and the heat exchanger network (between process-process as well as process-utility streams) rigorously considering the trade-off between efficiency and capital costs. Compared to the well-known HEN synthesis techniques, whether sequential or simultaneous, the proposed methodology allows to (1) select among several available utility systems, (2) include complex superstructures of utility systems (such as multiple-pressure-level steam cycles, heat pumps, refrigeration cycles, etc), (3) generate any possible match between process streams and utility streams (i.e., matches between process and utility streams are not necessarily placed at the hot/cold ends of the HEN superstructure), (4) configure and optimally design the utility systems and HEN simultaneously, taking into account of any possible synergy between process and utility streams. The proposed synthesis model combines the SYNHEAT temperature-stage HEN superstructure of Yee & Grossmann [1] with models and superstructures of utility systems. The resulting MINLP is more challenging than the original problem of Yee & Grossmann [1] due to the larger number of integer variables (not only for process stream but also for utility streams it is necessary to define an integer variable for each temperature stage) and nonlinear constraints. A two-stage optimization algorithm is specifically developed. The Variable Neighborhood Search (VNS) algorithm of Egea et al [2] optimizes the integer variables, and the SNOPT SQP algorithm optimizes the real ones. The two-stage code is tested on several literature HEN test cases, and on three heat integration problems involving both HEN and utility systems. Preliminary results show that the lower level SQP algorithm is extremely efficient (computational time < 0.05 sec), also on large-scale non-convex problems, and the VNS algorithm reaches close-to-optimal solutions in a few minutes, also on large-scale problems. However, further work is needed to improve the efficiency of the upper-level integer optimizer on large-scale problems, possibly evaluating different optimization algorithms and solution initialization strategies.

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[801]

Process Simulations Supporting a Techno-Economic Framework to Optimize the Biorefinery Supply Chains

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With the recent innovations in the field of renewable energy, several promising biorefining techniques have been discovered. While most of the techniques have demonstrated promising outcomes in a small scale set-up, validation of these for its practical viability must be substantiated. In the past, several state-of-the-art contributions have been documented in this field to estimate the impact of inherent uncertainties on the long term economic performance of a biorefinery. However, one of the major voids in the existing research is its ability to embody experimental details while identifying the optimum supply chain logistics. This contribution illustrates a novel methodology in capturing the experimental details and coupling it with a techno-economic framework. In order to develop the process simulations, various tools from the Aspen Engineering Suite are explored extensively and tailored in a unique manner to share critical data for further analyses. This attribute of the model enables successful linking of the basic sciences with the broad supply chain, guiding the decision making process. As a proof of concept, this research will demonstrate the applicability of the developed model for a biochemical conversion process to estimate the economic impacts of producing liquid transportation fuel. The resulting comprehensive framework will help channel resources appropriately and act as a decision support tool for investors, policy makers and related stakeholders.

[825]

A Rescheduling Algorithm for a Large-scale Reverse Osmosis Desalination Plant under Uncertain Fresh Water Demand

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The scheduling problem of a large-scale seawater reverse osmosis (SWRO) desalination plant is considered as a mixed-integer nonlinear programming problem (MINLP) over the time horizon. It is hard to find out the exact solution directly. Especially, when the working environment is changing, it is difficult to give the optimal solution in advance. So, when the situation is changed, it is need to find out a new scheduling plan quickly to meet the changes. In this paper, a rescheduling model of operational optimization of a large-scale SWRO is built, which is a bi-objective optimization with criterions of efficiency and stability. A rolling horizon scheduling (RHS) strategy is used to make the solution meet the requirement of accuracy and rapidity. The framework of RHS is structured and a two-stage differential evolution (TSDE) algorithm is used to compute the solution. A simulation based on a real case with fluctuations in freshwater demand in Liuheng Seawater Desalination Plant in Zhejiang province was made, and the results show that the performance of the proposed algorithm is satisfied.

[975]

Water Exchange in Eco-industrial Parks through Multiobjective Optimization and Game Theory

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The water exchange network problem of an Eco-industrial park (EIP) is addressed following two methodologies, namely multiobjective optimization (MOO) through goal programming and game theory. The problem is tackled using a mixed-integer linear programming (MILP) formulation and by solving the MOO problem using goal programming. First, the efficiency of goal programming for solving MOO problems is demonstrated with an introductive mathematical example of industrial water and energy networks design problem and subsequently, by applying the same methodology to the EIP water exchange network problem which formerly tackled in literature with other MOO methods1. Besides the mathematical model, EIP water exchange network problems entail several objective functions which are often antagonist between themselves, e.g., minimize operating costs of each enterprise involved. The solution of the MOO EIP water exchange network problem can be achieved in different ways, by for example, determining the Pareto front in its totality and choosing the trade-off solution a posteriori or by finding one trade-off solution a priori. In the former, several optimization problems have to be solved, while in the latter the solution is commonly narrowed to solve one or a few optimization problems. Nevertheless, EIP water exchange network problems may be very time-consuming or difficult to solve, since the number of variables (especially discrete) can be very large. This drawback is very limiting in the context of solving the problem by finding the Pareto front, since solution times for a single sub problem is often prohibitive by itself. On the other hand, a priori methods like goal programming, do not provide the entire Pareto front, although any solution found is inside it. The essential advantage is that the decision-maker preferences are included before the optimization. The case study is made up by an EIP containing 3 enterprises, each one with 5 processes. In this case only water exchanges are considered, and only one contaminant is assumed to be present in the network in order to maintain linearity in the model by making some valid assumptions. Regarding the regeneration units, the model takes into account the scheme to be adopted for the industrial park, i.e. shared/not shared regeneration units between enterprises.

In the game theory case, the problem is modeled as a bi-level optimization problem following the concept of "leader-follower", where the concept of EIP authority arises2. In fact, the EIP authority aims to minimize total freshwater consumption, while each individual enterprise aims to minimize its own total operating and capital cost. The methodologies proposed are demonstrated to be very reliable, in the case of MOO, by providing Pareto-optimal compromise solutions in significant less time compared to other traditional methods for MOO and in the game theory approach by applying a novel methodology for the design of raw matter/utilities network in EIPs.

[989]

Conceptual design of cost-effective and environmentally-friendly configurations for an integrated industrial complex

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An integrated industrial production complex with natural gas and locally sourced minerals as the main raw materials was studied. Elevenprocesses including a central synthesis gas plant which uses natural gas were examinedin optimization studies considering the exchange of materials and energy. The optimizationsincluded consideration of economics and environmental impacts as well asrobustness to unplanned production stops of individual processes. Materialbalances for the various chemical processes were built up based on data from literaturesources with the production scales assumed according to estimated market demandand economy of scale. The proposed industrial complex is aimed at an annualconsumption of natural gas around 2-5 billion Sm^3, which is assumed to besufficient for the landfall of a natural gas pipeline. Energy quantities andvalues of the streams in and out of the processes were also calculated and arepresented in the paper. The potential for material and energy savings byexchange between different processes is quantified by the flow-sheet. The optimizationis made using input data from the flow sheet in a Java-based MILP software(reMIND). Practical limitations, such as transportation, storage and technicalmaturity etc., have been included in the objective function for the model. Apartfrom improved economic profits, the cases are analyzed also with respect tocarbon dioxide emissions and energy requirement in the objective function. Dependingon the weightings applied to the objective function elements different optimal scenarioswere obtained. A sensitivity analysis of the response of the economic profit,energy consumption and CO_2 emissions to different operating conditions was alsoexamined.While there are benefits from the integration ofthe processes, the dependency between different plants also results in exposureto unplanned stoppages by connected processes. The allocation of benefits andliabilities between processes is reflected in a fair and transparent way byusing the model. Location specific factors are also included, particularlyidentifying the advantages (like heat recovery) and disadvantages (for example,transportation) and associated cost impacts from the localization in a coldclimate region.

[1002]

Modelisation of environmental impacts and economic benefits of Fiber Reinforced Polymers Composite Recycling pathways

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Composites are increasingly used in different applications (aerospace, automobile, industries, sports…) due to their high strength and lightweight characteristics. In aerospace, they have been used firstly in military aircraft for over 50 years. They have then progressively replaced metals in commercial aircraft in order to reduce operational costs. The recent models of Airbus (A350) and Boeing (B787) have employed large percentages of composites with more than 50wt% in which the majority is Carbon Fiber Reinforced Polymers (CFRP) [1]. The increase of utilization of CFRP has raised the environmental concerns on waste disposal and consumption of non-renewable resources as well as economic awareness for the need to recycle CFRP wastes. However, recycling of these materials is far from being a mature technology.

The aim of this study is to use process systems engineering methods to model the recycling pathways of two types of composites, i.e. Carbon Fiber Reinforced Polymers (CFRP) and Glass Fiber Reinforced Polymers (GFRP). Despite differences in fiber properties, the recycling techniques of these thermoset composites exhibit similar principles for recycling processes. In this work, mechanical recycling, pyrolysis and fluidized bed will be investigated and compared to other end-of-life solutions (incineration, co-incineration and landfill). A systemic approach is used to model the various options with the necessary degree of granularity to make the comparison consistent. The inventory, collection of all data on environmental emissions and costs, for the activities in the scenarios will be described together with the valuation of the environmental impact for the selected scenarios. The environmental effects are analyzed by application of Life Cycle Assessment, LCA. The objective is to quantify the gain obtained by material recycling, assuming replacement of virgin materials, as being the best choice in both economical and environmental terms which take into account the quality of the recycled fiber. Different scenarios will be studied by a sensitivity analysis in order to investigate the factors which influence recycling benefits. Results show that the choice of waste treatment strongly depends on the value of the materials input and on the recovered products. Transportation turns out to be an important factor to the environmental benefits of recycling. The next step of the proposed methodology will be to insert the waste management model for CFRP scrap into a multi-objective optimization model to determine the best options in a market wide perspective.

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[1018]

A MILP Transshipment Model to Integrate and Re-Engineer Distillation Columns into Overall Processes

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Energy integration has a pivotal role to secure maximum energy efficiency and sustainability of processes, since energy consumption has a great impact on the annualized total cost. Especially, distillation operations constitute a big share of the overall process energy consumption necessitating optimal energy efficiency. Further incentives for distillation re-engineering are related with the high majority of bioprocessing paradigms that appear particularly energy intensive separations due to enormous needs for water removal and the presence of numerous biological byproducts in downstream separations. In these cases, distillation energy consumption may range up to 80% of the overall energy cost. Multiple integration techniques, including thermally coupling, multi-effects, heat pumping etc, are used to optimize distillation energy efficiency. However, all these refer to individual column integration, independently the energy integration of the overall process [Linnhoff, 1983]. In this context, a mathematical systematic approach is demonstrated to retrofit distillation schemes according to integration of the whole process.

At a scoping stage, where multi-effect systems are used to recover distillation energy, there are fundamental designing challenges regarding the number of effects, operating pressures and distribution of distillation feed among them. Considering a set of candidate effects - operating at different pressures- numerous combinations can be generated, each of which represents a different distillation scheme. Under these circumstances, there are incentives to screen the various distillation schemes and detect the effects that are optimally integrated with the whole process. To integrate hot and cold streams of the process, an extended MILP transshipment model is formulated considering the utility needs of the candidate effects as additional degrees of freedom. As a result, it is possible to distribute the normalized heat contents of reboilers and condensers of the multiple effects along the process heat cascade and select effects and their capacities at appropriate operating pressures in the scope of minimum utility cost.

Capital and operating cost of the effects are additionally regarded during the optimization procedure to avoid multiplicities of solutions that arise from unnecessary selection of effects that do not offer lower cost of utilities.

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[1064]

A hybrid CP/MILP approach for big size scheduling problems of multiproduct, multistage batch plants

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This contribution presents an approach that uses the complementary strengths of Mixed-Integer Linear Programming (MILP) and Constraint Programming (CP) techniques to solve multiproduct, multistage batch plants scheduling problems that are otherwise intractable with either of these two methods. In particular, cases of high dimensionality, due to a great number of batches, are the target of the approach. The methodology has three phases. In the first one, an MILP model tackles the assignment problem – units are allocated to processing tasks. The second phase, which is addressed by means of a relaxed CP model, has a twofold goal: first, to check the feasibility of the previously obtained assignment, and second, to solve the sequencing problem taking into account sequence-dependent changeover times. When the assignment turns out to be unfeasible, cuts are generated and the first phase is solved again. The iteration between phases one and two continues until a feasible assignment is reached. In such a case, the third phase, which is a rigorous CP model that optimizes performance measures such as makespan, total or mean tardiness, etc., obtains the final solution. It is important to point out that the constraints included in the first phase of the approach allow, in many cases, to obtain feasible and efficient assignments, thus avoiding the need for iterations and reducing the required CPU time. The reduction of CPU time is also the reason for having both a relaxed (phase 2) and a tightened (phase 3) CP model, instead of just one, as in other hybrid CP/MILP methodologies. The approach has been implemented in the IBM ILOG CPLEX Optimization Studio (2014), in which both MILP and CP models can be defined. The approach accounts for many features that are found in industrial settings, such as forbidden batch-unit assignments, prohibited production sequences, various intermediate storage and interstage waiting policies, unit dependent processing times, order release times and due dates, finite unit ready times, as well as topology constraints, restrictions on renewable resources, like utilities, manpower, etc. In addition, production orders requiring several batches of each product can be fulfilled by operating in a campaign mode, as it occurs in many industrial facilities. When these campaigns are run, upper and lower bounds on the number of batches per campaign must to be complied with. The proposal has been extensively tested by means of several examples (60 to 200 batches) available in the literature (Kopanos et al., 2010; Castro et al., 2011; Authors, 2013). Numerical results show that for big-size cases, the approach can be faster than standalone MILP and CP models, and, more importantly, can solve problems that could not be solved with either of these methods alone. In addition, in many cases the quality of the obtained solutions is much better.

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[1102]

A Duality-based Approach for Bilevel Optimization of Capacity Expansion

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We address the problem of capacity expansion that maximizes the net present value (NPV) of an industrial gas company with multiple facilities, subject to markets that determine the company's income according to their own cost. The capacity expansion problem with a rational market resembles a strategic game in which companies establish their capacity expansion plans, and then the markets decide from which provider their demands are satisfied. We consider the strategic game with perfect information; the suppliers are aware of the decision criterion of the rational markets and the markets observe the actions of the suppliers before their decisions are made.

We formulate the capacity expansion problem with rational markets as a bilevel optimization problem. The upper level problem maximizes the leader's NPV and the lower level problem minimizes the cost paid by the markets. The decisions in the upper level problem are the investment related to capacity expansion, while in the lower level the markets decide whether they buy from the leader or from other providers. The lower level decisions are based on the economic interest of the markets and the prices offered by the different providers.

The resulting formulation is a mixed-integer bilevel linear programming (MIBLP) problem in which the upper level variables are mixed-integer, and the lower level variables are all continuous. In order to solve this problem, we consider a strategy that leverages the strong duality property of linear programs (LPs). In particular, the lower level LP is replaced by both its primal and dual constraints; strong duality is enforced with a constraint that equates the primal and dual objective functions. The complication of this approach comes from the nonlinearities that appear in the dual objective function of the lower level problem. These nonlinearities arise because the upper level variables are treated as parameters in the lower level. Therefore, the single-level reformulation includes the multiplication of upper level variables and lower level dual variables. However, the nonlinearities can be reformulated using exact linearization when all the upper level variables are discrete.

Two case studies from the air separation industry are used to illustrate the computational efficiency of the the Primal-Dual strategy. The expansion plan obtained from the bilevel formulation is also compared with the plan obtained from the standard single-level capacity expansion formulation. The results show that the single-level formulation yields higher investment cost because it overestimates the attainable market share. In comparison to the bilevel approach, such an expansion plan yields significantly lower NPV when evaluated in a rational market environment. These results clearly demonstrate the importance of considering markets' behavior to develop capacity expansion plans that are more robust in the dynamic conditions of the markets.

Maria-Ona Bertran, Thomas Bisgaard and Rebecca Frauzem (Eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. 31 May - 4 June 2015, Copenhagen, Denmark

Track 8. Enterprise-Wide Management and Technology-Driven Policy Making

[84]

Agent-based model of the German Biodiesel Supply Chain

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Complex adaptive systems refers to those systems whose overall behavior is extremely complex, yet whose fundamental components parts are each very simple, and constantly adapt to their environment. Examples of such systems are: Economies, ecologies, immune systems, the brain, and supply chains. Traditionally, supply chains (SC) have been modeled as a pure mathematical formulation (equation-based model). However, the interactions and inter-dependencies among different entities, processes and resources that make the SC a complex adaptive system are neglected (Surana, Kumara, et al., 2005).

Agent-based models are suitable to model complex adaptive systems. These systems are characterized for their distributed character (each actor/agent is to some extent autonomous); the agents operate in a highly dynamic environment; and the agent's interaction can be the result either from a reactive or pro-active attitude or from a propensity to co-operate or to compete (Helbing & Balietti, 2011).

In this work, the production of biodiesel from rapeseed in Germany was conceptualized using the complex adaptive systems (CAS) theory and formalized using the agent-based modelling approach. The agent-based model (ABM) incorporates farmer's decisions on market choice, and biodiesel producer's decisions on biofuel production and capacity expansion.

The aim of the agent-based model is to understand how different policies, either individually or collectively, have triggered: production of feedstock and biodiesel, and conversion capacity. The ABM was calibrated to replicate the pattern in the evolution of rapeseed, wheat, and biodiesel production in Germany in the period 1992-2012. It was found that complex adaptive systems theory could be used as a conceptual framework to analyse supply chains. In the specific case of biofuels supply chains, where it has been proven that exist due to subsidies and incentives from governments, the agent based modelling approach could be an important tool to analyse the impact of different policies on biofuels supply chains' performance.

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[97]

Decision Support by Multicriteria Optimization in Process Development: An Integrated Approach for Robust Planning and Design of Plant Experiments

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In process development, many decisions have to be made which involve finding compromises between conflicting objectives. In general, conflicting objectives can be weighted leading to one single objective. The according weights have to be known a priori and are usually fixed. Practical experience shows that this leads to a loss in optimization potential because usually some weights are uncertain orunknown. In Multicriteria optimization (MCO) no weights have to be selected. The set of best compromises, also known as Pareto set or Pareto frontier, is calculated and interactively presented to the designer. A decision is made based on navigating on this set and considering trade-offs between the objectives. MCO supports the designer in the decision process what has been shown before.The present contribution extends this scope to other tasks in process development: model adjustment, design of plant experiments and robust design under uncertainties. Software was developed which enables the use of MCO for solving these tasks. It is based on BASF's steady-state flowsheet simulator CHEMASIM.

In model adjustment, parameters of process models are determined by comparison of model predictions to experimental data from mini plants or production plants. Conflicts may occur when this adjustment is done for different operating points. In the literature, the model deviations of the different operation points are usually weighted by corresponding experimental variances following the theory of regression. In practice, however, these variances are often not given exactly. In this situation, MCO can be beneficially employed.

A sensitivity analysis reveals the influence of the parameters on selected output functions according to certain sensitivity measures. A sensitivity analysis alone does not provide a course of action if the sensitivity measures at the current operating point are outside the desired range. A remedy here again is a multicriteria point of view: Apart from objectives related to process performance like production costs or production capacity a suitable sensitivity measure is taken as a further objective which is to be minimized for robust process design or maximized for optimal experimental design.

This perspective offers several advantages compared to known approaches. The proposed approach has no restriction on the choice of sensitivity measures: They can be either local, i.e. partial derivatives, or global, like averaged difference quotients from a factorial design, elementary effects or partial variances, also known as sensitivity-based indices.

Results for several practical use-cases will be presented in the paper to demonstrate the benefits of MCO and the scope of the software.

[428]

A Study of the Sustainable Development of China's Phosphorus Resources Industry Based on System Dynamics

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As a non-renewable ore, phosphate rock is a very important strategic resource. However, in the process of the exploitation and utilization, there are severe waste and environmental pollution problems which are disadvantageous to the sustainable development of phosphorus resources. In order to promote the sustainable development of China's phosphorus resources industry, this research proposes a system dynamics model with two sub-models for thermal phosphoric acid and wet phosphoric acid separately, considering to the actual situation of regional phosphorus resources industry. This model focuses on industrial, financial, technological and environmental policies for the development of phosphorus resources industry, such as phosphorus resources exploitation, product structure adjustment, waste management and other policies. To find the optimum policy combination of sustainable development, the model which employs resource productivity, economic benefits, ecological efficiency and social satisfaction as objects, explores development situations of phosphorus resources industry and assesses the impacts of the policies by comparative policy scenarios. Results show that under the condition of excess capacity, optimization of phosphate fertilizer product portfolio is more advantageous compared with capacity expansion to increase production value of phosphorus chemical industry. And the combination of total consumption control policy of phosphate rock and acts to promote technical progress improves resource productivity. The implementation of waste recycling policies is conducive to improve continuously the eco-efficiency, and is not conducive to increase economic benefit due to more investment cost. Meanwhile, the public satisfaction is another key factor for the industry's sustainable development. Finally, this study indicates that an effective combination of total consumption control policy, product structure adjustment and appropriate environmental protection will be beneficial to the sustainable development of phosphorus resources industry. In addition, it contributes not only to the conservation of natural resources, but also to a reasonable disposition of the investment which can promote technological progress in industrial weak links. Moreover, the results can provide relevant references for policy makers to make appropriate decisions.

[944]

Interplant carbon integration towards phased footprint reduction target

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In order to limit dangerous climate change effects as a result of carbon dioxide build up in the atmosphere, policy makers are considering strict emissions targets. The introduction of such targets will require strategies to achieve them in efficient ways. Industrial parks or clusters can have significant carbon footprints, which may need to be cut drastically to allow national emissions targets to be met. For instance in Qatar, the country with the highest per capita carbon emissions, the energy industries together with the power and desalination sectors are responsible for more than half of national emissions. Systematic approaches for analysing carbon footprint reduction options in industrial clusters will be of great help in the development of strategies to cost effectively reduce footprints in support of national goals.

Carbon emissions reduction strategies for processing systems might aim at replacing energy sources, increasing energy efficiency, carbon utilization, or carbon capture and storage. Whilst the use of clean and renewable energy sources, energy efficiency and carbon capture and storage (CCS) has received much attention from the scientific community, little work has been disseminated to date on approaches to explore carbon utilization options. Carbon dioxide can be utilized in many different ways, including chemical or biological conversion into fuel, polymers, food supplements, fodder or another value added product. In addition, storing carbon dioxide underground might also create economic incentives to cut emissions in case of Enhanced Oil Recovery (EOR). The integrated analysis of utilizatiopn options together with the capture, separation, compression and transmission of carbon dioxide will be required to determine the most economically attractive footprint reduction solutions.

We present a systematic approach to integrate carbon dioxide within an industrial park with multiple carbon emitting streams and the potential carbon utilization options (sinks) that may exist. The approach identifies the lowest cost integration options to attain a given footprint reduction target and decides which sources are best captured together with their allocation to the various utilization options. It determines if the captured carbon dioxide should be purified and takes into account costs of carbon capture, carbon transportation between sources and sinks as well as costs associated with the utilization processes. It also takes into consideration the expansion of the industrial zone over time and determines the transition of the carbon source and sink allocations over the planning horizon to ensure compatibilty of solutions as overall emissions reduction targets are attained at different points in time.

The resulting multi-period planning problem has been formulated as an MINLP to determine minimum cost allocations and conversion of CO2 sinks into valuable products while considering carbon dioxide separation, compression and transportation in an industrial park setting. Targets for carbon reduction can be set for each time period and the problem is solved to yield optimal networks over time with consistent transitions between the periods. The approach will be presented together with a case study of an industrial cluster to illustrate the usefulness of the approach.

[1000]

Product and Process Network Modeling and Pathway Optimization with Life Cycle Functional Unit Analysis: The Case of Biofuels

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Biofuels are seen as a potentially viable source of liquid transportation fuels if they can be produced economically and in a sustainable fashion. This work develops a product and process model that integrates life-cycle assessment (LCA) impact objectives to optimize the economics and sustainability of a conversion pathway. Economic criteria considered include scaling capital costs with capacity, feedstock transportation costs, and operating costs. Life-cycle impacts considered include global warming potential (GWP), eutrophication potential, and smog formation potential. Profit is maximized as the economic objective, and the environmental objective is to minimize all negative environmental impacts. While the model can be adapted to a variety of technological sectors and pathways, this work focuses on bioconversion pathways.

The bioconversion network is composed of hundreds of technologies and compounds/materials and is the largest bioconversion technology network constructed to date. Data for the network was taken from various sources and previous technoeconomic analyses. A farm-to-use LCA is performed, taking into account biomass growth, harvesting, transportation, bioconversion processing, and final product transportation and use. Environmental impact factors and inventories were compiled from Argonne's GREET™ model, and NREL's U.S. Life Cycle Inventory Database [1,2]. Altogether, the network is modeled by a nonlinear program (NLP) that is approximated by a branch-and-bound algorithm using piecewise linear approximations. The proposed algorithm reproduces results of off-the-shelf global solvers in less time.

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Track 9.1. Molecular Systems Engineering

[184]

Molecular dynamics simulations with all-atom models for a detailed understanding of protein dye-affinity interaction

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Dye-ligand affinity chromatography has been widely used in protein separation and purification. Immobilized textile trazine dyes, particularly Cibacron blue have been used as affinity chromatography tools for a long time. The advantages of Cibacron blue as affinity ligand include its low cost, ease of immobilization, resistance to biological and chemical degradation and high protein-binding capacity of the corresponding adsorbents. Cibacron blue interacts with a large number of seemingly unrelated proteins. This endows Cibacron blue with a serious drawback of compromised protein binding specificity. To cope with this drawback and improve the application of Cibacron blue in protein separations, a better understanding of the interaction mechanism between Cibacron blue and different proteins is necessary. Since Cibacron blue has a special chemical structure, its binds with both hydrophobic and hydrophilic parts of the proteins. Several factors affect the interaction between Cibacron blue and the proteins, such as pH, ionic strength and the density of immobilized ligands. The understanding of these influences is also important in understanding the interaction mechanisms.

In this presentation, molecular dynamics simulations with all-atom models are applied to investigate the interaction of Cibacron blue with two proteins at different pH values in detail. Molecular dynamics simulation provides clear and direct microscopic information, which has been successfully used in our former research on the ion-exchange chromatographic adsorption processes of proteins (Liang et al., 2012). The interactions between Cibacron blue and two different proteins, serum albumin and hemoglobin, at different pH values are simulated and analyzed. All-atom models of these affinity interaction systems were applied for a precise study. The interaction mechanism as well as the binding sites of proteins at different pH values will be analyzed on a molecular scale. Moreover, the simulations of these two different proteins will be compared systematically to explore the specific mechanism. These simulation results will be compared with the former experimental results as well. The results of this presentation are the basis for a better understanding of the interaction between Cibacron blue and different proteins, which can be used to guide the choosing of effective specific eluents in protein separation, the design of new dye-ligands with improved affinity and specificity, as well as the optimization of dye-ligand affinity chromatography.

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[230]

Steady-State Monte Carlo Simulation of Microstructural Distributions for Copolymerization Processes on a CUDA Platform

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Polymers can be used in diverse applications in daily life because of their various microstructures. Thus, microstructural distributions are of great importance for evaluating the quality of polymer products. Monte Carlo simulation is an efficient method for obtaining certain microstructural distributions that cannot easily be determined by traditional equation-based methods. This simulation, however, suffers from the drawback of requiring long computation times. In this paper, a parallel method is proposed for the steady-state Monte Carlo simulation of the microstructural distributions for copolymerization processes on a CUDA platform. The computation time of the proposed method is greatly decreased by at least tenfold compared with the time required by traditional CPU platforms. A case study is also presented to show the accuracy and efficiency of the proposed method.

[558]

Computer-aided design of solvents for the recovery of a homogeneous catalyst used for alkene hydroformylation

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Recent works have demonstrated the use of thermomorphic solvent systems (TMS) in the recovery of homogeneous catalysts, especially for the hydroformylation of long-chain alkenes such as 1-dodecene [1]. In this case, this special TMS mixture was comprised of dimethylformamide and decane; however, these solvents were not rigorously screened and may represent a suboptimal solution for catalyst recovery. Also, in view of other homogeneously catalyzed reactions, a systematic approach to solvent selection for catalyst recycling is desirable. In this contribution we propose using an approach similar to those practiced in the pharmaceutical industry for predicting the solubility of APIs in different solvents. In this manner, two different computational methods were compared: (1) a predictive model using the Conductor Like Screening Model for Real Solvents (COSMO-RS) model [2] to screen solvent mixtures and (2) an NLP formulation based on the semi-predictive Non-Random Two-Liquid Segment Activity Coefficient model (NRTL-SAC) [3] to find optimal solvent mixtures. In order to use NRTL-SAC, segment parameters of the catalyst had to be fit to solubility data in various representative solvents. After two different sets of candidate solvent mixtures were identified using both procedures, the separation characteristics of these solutions were determined experimentally in order to evaluate the feasibility of each method for use in process-wide design.

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[764]

Computational Molecular Design of Water Compatible Dentin Adhesive System

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The objective of this work is to develop a framework to a design dentin adhesive system for water compatibility and efficient photo-polymerization applying computer aided molecular design. A dentin adhesive system consists of monomers and photo-initiators which trigger a photo-polymerization reaction when exposed to visible light. In this study a water compatible visible light photosensitizer was designed for dental applications. Quantitative structure property relationships (QSPRs) were developed for relevant properties (octanol/water partition coefficient and molar extinction coefficient) using molecular descriptors. The QSPRs are combined with structural constraints to form a mixed-integer nonlinear problem (MINLP), which is then solved to near optimality using Tabu search to generate novel candidate photosensitizer molecules with desired properties. Tabu search, a heuristic optimization method, does not yield globally optimal solutions for MINLPs, but it is an efficient and practical method for solving general combinatorial optimization problems. This framework will provide insight regarding possible functional groups for developing water-compatible visible light photosensitizers for dentin adhesive systems.

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[1092]

An Evaluation of Thermodynamic Models for the Prediction of Solubility of Phytochemicals from Orthosiphon Staminues in Ethanol

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Orthosiphon Staminues (O.Staminues) is a species of herbs locally known in Malaysia as Misai Kucing. It has been used by the traditional medical practitioners to treat joint inflammation, gout, arthritis, rheumatism and remedy for kidney stones (Pouralinazar et al., 2012, Yam et al., 2010). This study aims to develop a Group Contribution-based (GC) model to determine the solubilities of biomarker compounds from O.Staminues. The biomarker compounds are sinensetin (SEN), eupatorin (EUP), 3-hydroxy-5,6,7,4-tetramethoxyflavone (TMF), and rosmarinic acid (Akowuah et al., 2004) which have been accepted as having properties of pharmaceutical importance. The solubility predictions of the biomarker compounds in two solvents using the developed UNIFAC-based GC model were compared with the predictions made by the NRTL-SAC (Tung et al., 2008, Chen and Song, 2004) and Original UNIFAC model (Fredenslund et al., 1975). The solvents studied were water and ethanol. The solubility experimental data were taken from the literature, whereas the missing data were determined by solubility experiments via the analytical isothermal shake-flask method. Using our developed GC-based model for O.Staminues, better agreements between the experimental and predicted values, and much lower deviation errors were obtained as compared to the NRTL-SAC and the Original UNIFAC model. The better results can be due to the fact that the GC-based model proposed in this work was developed based on the herbs data comprising of biomarker compounds with more complex structure as compared to the original UNIFAC model which was based on simpler molecules. The UNIFAC-based GC model can be useful for solubility estimations of biomarker compounds of O. Staminues in various solvents.

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[1130]

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

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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 approached 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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[1145]

Quantum mechanics simulations from fundamental binding energy to solvent evaluation tool: A case for benzene-cyclohexane separation

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Separating benzene and cyclohexane is difficult, because they form an azeotropic mixture and have similar boiling points. Therefore, separating the mixture requires extractive distillation. This study evaluated for a more effective solvent using a quantum mechanics (QM) simulation method – density functional theory (DFT) to calculate binding energy (EBsolvent), binding constant (Ksolvent) and fitting value (X) for each solvent. From the simulation, the five most appropriate solvents for separating benzene from cyclohexane, in order of effectiveness, were: morpholine > N-formylmorpholine > methyl sulfolane > sulfolane > propyl formate. Our QM solvent evaluation method agreed well with experimental results, making it as a powerful tool for solvent evaluating and more effective solvent extractive distillation.

Track 9.2. Biological Systems Engineering

[182]

Mathematical analysis of multistage population balances for cell growth and death

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The cell cycle is a biologically timed process by which cells duplicate. It consists of 4 phases, during which cells undergo different mandatory transformations. Modelling the cell cycle therefore requires capturing the evolution of those processes inside of each phase. This can be formulated in terms of cell age or cell content (mass/volume) and they can be univariate or multivariate. The cellular heterogeneity is therefore an intrinsic feature of all cell systems, ranging from the genetic level to the culture environment level. An underlying source of such heterogeneity is the cell cycle segregation for both industrial [1] and clinical applications.

The multistage population balances can better describe the physics of cell cycle progression through phases than lumped growth models. These balances can be formulated in terms of cell age/mass/volume (difficult to experimentally quantify) or cell content (relevant markers are required) and they can be univariate or multivariate. A specific, biologically-relevant, three stage population balance model has been recently proposed to simulate evolution of several cell cultures is studied here in detail [2]. The three governing equations of this model are composed by growth and transition terms. In this work the relation between the multistage Population Balance (PB) model and the corresponding lumped model is discussed in detail. It is shown that the lumped model can be derived by considering uniform content distribution in the cells or at the limit of coarse discretization of PB model. The two models can give similar results though using different set of parameters. A one equation analog of the multistage model is formulated and it is solved analytically in the self-similarity domain. The effect of initial conditions at small time is studied numerically. Exact results are given for the relation between growth and death parameters of the PB and lumped models. The three model equations are then considered by using asymptotic and numerical techniques. It is shown that in the case of sharp inter-stage transition the discontinuities of the initial conditions are preserved during cell growth whereas for distributed transition the cell distribution converges to a self-similar (long time asymptote) shape. It is also illustrated that the closer the initial condition to the self-similar distribution, the faster the convergence to the self-similarity and the smaller the oscillations of the total cell number. The findings of the present work leads to a better understanding of the multistage PB model and to its more efficient use for the understanding and use experimental data for model-based application studies.

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[292]

Oxygen transfer rates and requirements in oxidative biocatalysis

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Oxidation reactions are widely applied in the chemical industry. However, conventional chemical oxidation suffers from limited selectivity and high environmental impact, due to the use of (often chlorinated) organic solvents, transition metal based catalysis or stoichiometric amounts of inorganic reagents [1]. Biological catalysts offer the possibility to perform highly regio- and stereo selective oxidation reactions using molecular oxygen as electron acceptor, hence avoiding chemical waste generation. The biocatalyst can either be in the form of soluble enzyme or whole-cells (resting or growing microbial cells), depending on the type of enzyme and choice of cofactor regeneration system. Soluble enzymes require oxygen only for the oxidation reaction, whereas whole-cell catalysts also require oxygen to sustain cell maintenance and eventual growth. Thus a successful biooxidation with the intended space-time yield requires sufficient oxygen transfer to the bioreactor, which potentially could become a problem at industrial scale.

The method of oxygen supply needs thorough consideration. Depending on the biocatalyst (whole-cell or soluble enzyme), different techniques may be applicable. For example, the presence of a gas-liquid interface (bubbling) is known to cause inactivation of formate dehydrogenase (FDH) and laccase used for co-factor regeneration in biocatalytic oxidation reactions [2,3].

By applying a metabolic model based on flux balancing it is possible to predict and compare the oxygen requirements of growing cells, resting cells, and soluble enzymes catalyzing biooxidation reactions. The process model requires the input of energetic requirements of the microbial strain, specific activity of the biocatalyst, concentration of the biocatalyst, and specific growth rate of the cells. Based on experimental values reported in the literature the oxygen requirements of several biooxidation processes have been calculated and compared with the typical oxygen transfer capabilities of industrial scale bioreactors in order to evaluate if oxygen requirements will be limiting the reaction upon scale-up.

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[302]

Theoretical and Experimental Analysis on Biogas Production

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The research shows comparison of theoretical and experimental work to validate the thermodynamics of biogas production process. At the end of the experiment, the results show the best substrate and temperature conditions for biogas production. The effect of water content and pH in the digester is also analysed. The maximum methane concentration in the gas produced is obtained. The results also show the relationship between methane produced and the amount of substrate fed. A close analysis of the bacterial present in the digester shows that a number of bacterial is responsible for the production of biogas under anaerobic conditions.

[325]

Robust process design for the bioproduction of β-carotene in green microalgae

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Secondary metabolites from marine origin are of high commercial importance for the production of nutritional, pharmaceutical and cosmetic additives. Dunaliella salina is among the most extensively studied microalgal species, because of its ability to over-accumulate beta-carotene under environmental stress conditions, e.g. under high irradiance and depletion of nutrients present in the form of nitrate.

Currently, natural beta-carotene is mainly produced in batch cultivations in outdoor operation systems. However, these systems are typically designed and operated rather on an empirical basis. A profound understanding of the operating process including the impact of the uncertainties due to environmental fluctuations and biological variability is largely missing. Indeed, such uncertainties could have a large impact on process yield and stability especially in view of up-scaling from lab- to large-scale outdoor cultivation scenarios.

In this work, we present a probabilistic model-based process design and analysis tool. We use a hybrid uncertainty propagation strategy approach based on sigma point and profile likelihood sampling, e.g. [1,2], to account for the nonlinear propagation of uncertainties in operating conditions and model parameters. The design approach is illustrated using a dynamic-kinetic bioprocess model of Dunaliella salina in the form of ordinary differential equations (ODEs) [3]. This model describes growth and pigmentation in a semi-mechanistic way, and covers the main aspects of (i) light attenuation in the bioreactor and (ii) nutrient uptake of the cells, which both are key factors for carotene accumulation. The results of this work pave the way to the systematic analysis and robust design of efficient bioproduction processes under uncertainties due to environmental and biological variabilities.

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[338]

PSESP: Process Systems Engineering of Seeds Production

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High yielding and low variability production of high quality seeds is an essential component for future food security.

Most seeds production unit operations are related, but not identical, to those in the chemical industry. Indeed seeds, as a material, have different characteristics from chemical compounds and this leads to specific analytical techniques and differentiated production targets.

The scientific literature on seeds processing is not as mature as that available for chemical operations. Nonetheless, chemical engineering fundamentals can still be adapted within a systems framework to yield useful insights and optimize both production and process development. As a result the objectives of seeds process modelling are not only generic, transposable and scalable models but, perhaps more importantly, the understanding they provide.

The technical approaches and targets for engineering investigation are delineated within a framework of linked unit operations, relative importance for product quality and cost, and available science and technology. The relative value, and ease, of implementation naturally lead to proposals for further work.

[390]

Dynamics and Operation Analysis of the PHB (Polyhydroxybutyrate) Fermentation

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Biorefineries are mostly known for the production of energy, but the production of some biomolecules of interest and other biomaterials are also integrated. They require complex production process engineering tools for design, analysis and optimization, in order to include important factors such as low production costs, high yields and a process that is environmentally friendly. A variety of organic chemicals can be obtained from sustainably use of renewable raw materials. For instance the production of PHB (polyhydroxybutyrate), which belongs to the group of PHA (polyhydroxyalkanoate) that is a biodegradable polymer belonging to the polyesters class [1]. This biotech product is gaining importance worldwide due to their applications such as packaging materials, boxes, fiber and foam materials, medical implants, and carriers for drug delivery among others.

In general, the production of PHA granules is promoted due to unfavourable conditions for the growth of bacteria. These biopolymers are produced and accumulated inside the cell as energy reserve when the bacterial cells are under stress (as limitation of nutrients) and an excess of carbon source. It has been reported that it can be reached in bacteria up to 80% of its dry weight in PHA molecules [2]. Currently the main problem, which limits the widespread use of PHB, is its relatively high cost compared with polypropylene. The fermentation process, substrates and product recovery are the major cost. Several studies have tackled this problem using different approaches, focusing mainly on the kind of microorganisms and substrates, as well as on the process configuration design and optimization. However for most multivariable processes, in which numerous potentially influential factors are involved, it is not always obvious to determine which are the most important. Hence, it is necessary to submit the process to an initial screening design prior to optimization and control.

In this study, sugarcane molasses (a by-product of the sugar refinery industry with over 50% sugar content) is used as substrate for the PHB fermentation by *Azohydromonas lata* [2]. The objective is to study the process dynamics and to determine the influence of operating conditions for PHB fermentation process, using modelling and simulation tools. A dynamic model of the isothermal reactor fermentation (either batch or fed-batch mode) is used to obtain mainly product yield and productivity, analyzing the effect of operating conditions (e.g. operation mode, substrate concentration, fed considerations, nutrient concentrations, etc.). Results will be used in the short term for process optimization, as well as economic and environmental analyses.

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[421]

Exploring Opportunities for the Production of Chemicals from Municipal Solid Wastes within the Framework of a Biorefinery

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The unregulated disposal of organic fraction of municipal solid waste (OFMSW), or biowaste, can lead to health risks and the production of greenhouse gases, if not properly managed. Common treatment technologies aim at stabilizing the OFMSW by either oxidizing the readily degradable organics (e.g. composting), or converting them into reduced end products such as biogas or ethanol. Currently, the emphasis has been on optimizing the conversion of the OFMSW to these final products. However, advances in biomass based biological and catalytic engineering have let the conversion of the OFMSW to value added chemicals seem more appealing. Yet, the OFMSW cannot be used directly for these processes, but needs to be converted to intermediates. This study aims at assessing the economic opportunities of producing such intermediates from OFMSW within the framework of a biorefinery. A computer-aided collaborative environment, constructed in Aspen Plus, offers the essential evaluation platform. The purity and composition of the intermediates, as well as the estimation of the operating costs for the associated processes, can serve researchers, working on the production of value added chemicals from biomass, in assessing the feasibility of their proposed processes, using OFMSW derived intermediates. The OFMSW was chosen as the feed because of its low cost and reliable availability throughout the year especially in arid regions like Abu Dhabi.

The fundamentals of this study will be illustrated through the scope of two platforms, which are used for the production of essential intermediates that can feed the manufacturing of a broad range of chemicals. The first platform involves enzymatic hydrolysis for the production of sugars, and the second platform involves dark fermentation to produce volatile fatty acids (VFAs). In the first platform, OFMSW undergoes physical pretreatment followed by enzymatic hydrolysis to form intermediates. These intermediate compounds are sugar derivates which can be used in other catalytic or biological processes, to produce value added chemicals. The residue from the process can be used as a fertilizer or fodder for animals, depending upon its composition. In the second platform, which uses dark fermentation, a mixed microbial culture converts the sugars, proteins and lipids present in OFMSW to a mix of dilute volatile fatty acids (VFAs),H2 and CO-2. The process is simple and cost efficient, but product composition is hard to control and suppressing methanogens that scavenge products remains a challenge. The residual biomass can be separated, composted and sold as fertilizer. The dark fermentation effluent can be used directly in a biological downstream process after a small pretreatment. Alternatively, distillation can be used to take advantage of the azeotropes that only few VFAs form with water, to obtain a more defined intermediate stream.

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[475]

Development of a Macroscopic Model for the Production of Bioethanol with High Yield and Productivity via the Fermentation of Phalaris aquatica L. Hydrolysate

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The utilization of bioethanol has recently attracted worldwide attention as the means for reducing greenhouse gas emissions and improving global energy security. 2nd generation biofuels, derived from the bioconversion of wood and crop residues, energy crops and municipal wastes, can serve as direct complementary fuels for transportation. Phalaris aquatica (L.) is a perennial herbaceous energy grass with high carbohydrates content and biomass production capabilities, suitable for cultivation in marginal farmlands, presenting low nutrients and water demands. Thus, it constitutes an excellent energy crop and lignocellulosic biomass feedstock, serving as an abundant source of natural sugars which can be fermented to bioethanol.

In the present work, an integrated bioprocess for the production of bioethanol from P. aquatica lignocellulosic biomass has been developed and optimized. The process consists of three distinct stages that were designed and optimized under statistical experimental analysis: i) dilute acid pretreatment of the dried biomass for hemicellulose hydrolysis, ii) enzymatic saccharification of the residual solid fraction (i.e., cellulose) for glucose production, and iii) fermentation of glucose monomers for bioethanol production. The development of an accurate model representation of the process dynamics of the fermentative bioethanol production stage is a prerequisite for the optimal operation and control of the bioprocess. In this context, a macroscopic mathematical model has been developed to quantify the production of bioethanol in Saccharomyces cerevisiae cultures. In particular, the model qualitatively and quantitatively accounts for biomass growth, intracellular bioethanol production and excretion and carbon consumption rates, taking into account substrate and product inhibition phenomena. The predicted capabilities of the proposed model were assessed by a direct comparison of the model predictions with experimental data, obtained from a series of batch and fed-batch cultivations in flask and bioreactor cultivation scales.

The process model and experimental results demonstrated the production of bioethanol with increased yield (up to 98.1% of the theoretical maximum value) under batch conditions. On the other hand, the bioethanol concentration and overall production rate were optimized (61.7 g/l and 2.42 g/(l·h), respectively) through the investigation of different feeding policies (i.e., constant and exponential) under high initial substrate loading. The present dynamic model succeeded in elucidating the role of key bioprocess variables and quantitatively describe their effects on the production of bioethanol in a 2nd generation biorefinery concept.

[480]

Enzymatic Reactive Distillation for the Transesterification of Ethyl Butyrate: Model Validation and Process Analysis

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For the production of new and more sustainable products, new technologies need to be developed. Within process intensification, reactive distillation which is the integration of reaction and distillation in one apparatus is one known technology. A new concept is to integrate enzymes into the distillation column which enables new or more selective reaction routes. However, matching operating windows is difficult due to for example the temperature sensitiveness of the enzyme. Here, modeling is an important tool for design, scale-up, analysis and optimization of chemical and biochemical processing by enzymatic reactive distillation systems. The lipase-catalyzed transesterification of ethyl-butyrate with n-butanol is highlighted, which is an equilibrium-limited reaction. Based on kinetic data and investigations of a surface coating to provide the enzyme into the reactive section, a detailed model of a continuous enzymatic reactive distillation is developed in Aspen Custom Modeler®, including hydrodynamic and mass transfer investigations of coated reactive packings. Subsequently, the detailed model is validated against experimental data of a pilot-scale enzymatic reactive distillation column with a diameter of 50 mm to check the agreement between experiments and modeling.

[584]

Design of a Gene Metabolator under Uncertainty

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This work aims to optimally design a metabolator, which is a metabolic process of Acetyl Co-Enzyme A (Acetyl-CoA) and its co-factors, with a view to incorporate uncertainty. The metabolic process can be described using a dynamic model involving nonlinear differential equations. An artificial neural network (ANN) transformation is utilised in order to transform the dynamic model of the metabolator into a system of simultaneous algebraic equations. The metabolator simulation problem is first solved and then the design problem is formulated as an optimisation problem, where the objective is to control the concentrations of Acetyl-CoA at desired set-points by manipulating the glycolytic flux. A non-linear model predictive control (NLMPC) formulation is then presented for computing the value of the source energy for the system, the glycolytic flux, which is used as the control variable. In this work Zone NLMPC is used to address the effect of uncertainty in the glycolytic flux as the system is allowed to perform within a range rather than at a fixed set point.

[604]

Manufacturability Indices for High-Concentration Monoclonal Antibody Formulations

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The need for high concentration formulations for subcutaneous delivery of therapeutic monoclonal antibodies (mAbs) presents manufacturability challenges for the final ultrafiltration/diafiltration (UF/DF) step. Viscosity levels and the propensity to aggregate are key considerations for high-concentration formulations. As a result it is critical to choose the optimal formulation for both efficacy and manufacturability in terms of being able to process the material in the final UF/DF step. This work presents a set of manufacturability indices related to viscosity and aggregation as early predictors to rank high-concentration mAb formulation conditions in terms of their ease of manufacture. Advanced multivariate analysis techniques are used to analyze published experimental DoE (design of experiment) data from industry that explores the influence of different formulation conditions (pH, ions and excipients) on the solution viscosity and mAb thermostability. A decision tree classification method, CART (Classification and Regression Tree) is used to identify the critical formulation conditions that influence the viscosity and thermostability. Polynomial regression techniques combined with the impact of protein concentration-time profiles and flux decay behavior during UF/DF are used to transform the DoE data into a set of stress maps which show viscosity and thermostability as functions of the formulation conditions and time profiles during final UF/DF step. Manufacturability indices are derived from analysis of the stress maps and the process conditions experienced in the final UF/DF step. The indices are used to identify the optimal formulation conditions that minimize the potential for both viscosity and aggregation issues during final UF/DF step. This approach can be used early in development to rank different formulation conditions for high-concentration product in terms of their ease of manufacture.

The viscosity stress maps for different formulation candidates capturing time exposed to different viscosity levels in UF/DF step are visualized. Different colors indicate different viscosity values (cP). The viscosity index for each candidate (in white numbers) indicates the average viscosity value of the product stream during the UF/DF step taking into account the time profiles of pH and concentration. Each set of formulation conditions can be ranked according to their viscosity indices where a low index value indicates a more desirable outcome.

[678]

Estimating Nonlinear Infectious Disease Models with both Discrete and Continuous Parameters

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Parameter estimation plays an important role in the understanding of infectious disease dynamics and decision-making in public health. Recently, optimization-based approaches have shown encouraging results and provide computational benefits by estimating unknown disease parameters with nonlinear dynamic optimization techniques. Many of the techniques used in this area provide only locally optimal solutions, or no guarantee of optimality at all. Furthermore, these strategies have been applied to deterministic and stochastic models based on continuous parameters only, while important effects like seasonality may be best represented using discrete variables. The major contribution of this work is twofold.

The well-known discrete time-series susceptible-infected-removed (TSIR) disease model contains several parameters, including a time-varying parameter to represent seasonality in the transmission rate. The original TSIR model is a special case of Yule process and the number of infectious individuals over time is governed by a negative binomial distribution. With this assumption, the parameter estimation problem can be formulated as a maximum likelihood problem and solved using mathematical programming techniques. Frequently, no functional form is assumed for the seasonal transmission parameter (other than periodicity from year to year), and the estimation formulation is a large-scale nonlinear programming (NLP) problem. For seasonality induced by school-term holidays, however, a more appropriate representation is to impose an on/off switching pattern in the transmission parameter, which gives a mixed-integer nonlinear programming (MINLP) problem.

In previous studies based on local optimization techniques we have found multiple local minima in the parameter estimation problem. Not all of these local minima produce parameters that are consistent with epidemiological understanding of the system. For this reason, it is important to solve these problems to global optimality and verify that the parameters estimated from the time-series data are consistent with other estimated (e.g. from age-based data). In this work, we make use of global optimization techniques to solve these parameter estimation problems. Based on a log-transformation, we reduce the nonlinearity to univariate functions that can be handled with outer approximations produced from linear under-estimators and piece-wise linear over-estimators. Typical bound tightening strategies, such as optimality-based bound tightening (OBBT) and feasibility-based bound tightening (FBBT) are applied. This strategy is successfully applied to both the NLP and the MINLP formulations and solution times are compared with off-the-shelf global optimization tools. Computational results are shown based on real case-count data from three different cities. The estimated on/off switching patterns obtained by solving the MINLP problems are strongly correlated to school term holidays across very different social settings and holiday schedules.

[829]

Experimental validation of in silico flux predictions from a genome-scale model (iMM518) for carbon dioxide utilization by M. maripaludis

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Increased use of fossil fuels worldwide encourages the production of chemicals and fuels from CO2 fixing microbes. M. maripaludis, a hydrogenotroph, is capable of reducing CO2 to methane in the presence of electron donors such as H2 or formate. To explore the metabolic potential of M. maripaludis for CO2 conversion to methane, it is crucial to quantify its substrate uptake and methane production rates. While genome-scale models are very helpful in studying intracellular and extracellular fluxes in the metabolism of a microorganism [1], validating the model predictions with experimental measurements is extremely important.

In this work, we perform a dynamic cell growth study in a batch culture of M. maripaludis and estimate three key extracellular fluxes, namely CO2 uptake, H2 uptake, and CH4 evolution for different growth rates. To the best of our knowledge, this is the first study to report CO2, H2 consumption and CH4 production rates under an environment where CO2 is the sole carbon substrate. We present a rigorous process simulation approach for estimating such fluxes from experimentally measured compositional data. Using the same data, we also present an approach to estimate Non-Growth Associated Maintenance (NGAM) energy required for cell survival, and Growth Associated Maintenance (GAM) energy required for growth. We then use iMM518, a genome-scale model for M. maripaludis [2], to predict the extracellular fluxes (mmol/gDCW-h) and compare the predictions with measured values. Finally, using the validated iMM518, we analyze the distribution of carbon flux between central metabolism and methanogenesis.

Exceptionally high uptake and production rates were observed in M. maripaludis with a high growth yield. Based on the results, M. maripaludis is capable of reducing 70-95% of CO2 to methane during exponential phase. This study shows the predictive power of iMM518 and helps us investigate the intracellular metabolic profiles underlying the extracellular observations.

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[1107]

Computer-Aided Process Analysis of Perillic Acid Production via Biocatalytic reaction

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Currently, the implementation of scalable biocatalytic processes often requires the introduction of process and/or biocatalyst enhancements to ensure effective scale-up.

This work describes an approach for evaluating biocatalytic processes in an early-stage of development from a process design, economics and sustainability point of view, in order to provide guidance on process and biocatalyst modification.

This approach is illustrated with a case-study – the biocatalytic synthesis of R-(+)-perillic acid by Pseudomonas putida DSM 12264. Perillic-acid is a monoterpenoic acid with a broad growth-inhibitory effect on bacteria, yeast and moulds, which makes it an attractive candidate to be used in substitution of conventional preservatives, particularly in cosmetic industry [1].

Process simulation and modelling on the commercial simulation software SuperPro Designer® are used as a tool to evaluate different scenarios.

Additionally, the impact of single input variables was studied by sensitivity analysis, which allowed the identification of key parameters for process development and targets for critical process metrics, such as product concentration (gproduct/L) and space-time yield (gproduct/Lreactor/h).

Based on this early-stage process analysis, guidelines for biocatalyst and process development were made, which can guide process development, assist research and support decision-making.

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[1128]

Ozonation of antibiotic in a microreactor

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Over the past few years, antibiotics have been considered as emerging pollutants due to their continuous input and persistence in aquatic ecosystem even at low concentrations. They have been detected worldwide, indicating their ineffective removal from wastewater using conventional treatment methods. In this study ozonation as a method for decomposition of antibiotic (Amoksiklav®) was applied, where continuous monitoring of antibiotic degradation with in-line HPLC analytics was employed. Microreactor technology demonstrated to be very effective method for removal of antibiotic with ozone with excellent process control. In this work Y-shaped microchannel with dimensions 100 μm x 205 μm x 12.5 mm regarding depth, width and length, was used for the ozonation process at residence times ranging from 10 - 100 ms. In a single flow through the microreactor system for a given geometry, a 67 percent of antibiotics inlet concentration is degraded at residence time of 100 ms. Furthermore, a mathematical models with full 3D description of transport phenomena, incorporating convection, diffusion and reaction terms along with the parabolic velocity profile, was developed to simulate the concentrations of process variables inside the microchannel, and to optimize the ozonation process at the micro scale.

Track 9.3. Pharmaceutical Systems Engineering

[176]

Cell cycle model selection for leukemia and its impact in chemotherapy outcomes

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The cell cycle is the biological process used by cells to replicate their genetic material and give birth to new cells that are in turn eligible to proliferate. It is highly regulated by the timed expression of proteins which trigger cell cycle events such as the start of DNA replication or the commencement of mitosis (when the cell physically divides into two daughter cells). Mathematical models of the cell cycle have been widely developed both at the intracellular (protein kinetics) and macroscopic (cell duplication) levels. Due to the cell cycle specificity of most chemotherapeutic drugs, these models are increasingly being used for the study and simulation of cellular kinetics in the area of cancer.

In this work, we present a population balance model (PBM) of the cell cycle in leukemia that uses intracellular protein expression as state variable to represent phase progress. Global sensitivity analysis [1] highlighted cell cycle phase durations as the most significant parameters; experiments were performed to extract them and the model was validated [2]. Our model was then tested against existing models of the cell cycle (ODEs, delay differential equations) in their ability to fit experimental data and oscillatory behaviour. We subsequently coupled each of them with a pharmacokinetic/pharmacodynamic model of chemotherapy delivery that was previously developed by our group [3]. Our results suggest that the particular cell cycle model chosen highly affects the outcome of the treatment, given the same cell cycle parameters and drug dosage/scheduling, with our PBM appearing to need the lowest dosing of drug for the same cell killing. Lastly, we show how varying cell cycle parameters (using the same PBM model) can dramatically affect chemotherapy outcomes, and the significance of this finding in the area of personalized treatments and prognosis grouping in leukemia.

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[248]

PAT for in-depth understanding and process design for crystallization of active pharmaceutical ingredients

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Many active pharmaceutical ingredients (APIs) are capable of forming different solid forms (polymorphs and/or hydrates). With the increasing number of poorly water soluble drug candidates, a metastable solid form might be selected for the final product development due to its preferred physiochemical properties, such as the aqueous solubility and dissolution rate. As a consequence, a robust and reliable crystallization process needs to be designed and developed to produce the selected solid form of API with the desired product property attributes. The design and development of such selective crystallization process requires in-depth understanding of the nucleation mechanism at molecular level and the comprehending of the process parameters' effect at process level. Nucleation of molecules into solid nuclei is the start of the process and plays an essential role in determining the kinetics of the process, as well as the molecular level structure and the particulate characteristics of the crystallized solid substance. However, nucleation remains as a poorly-understood and mysterious process for many years due to its complex nature. The essential difficulty of studying nucleation includes the size of the newly formed nucleus and the time scale of forming a nucleus. In the present work, crystallization of the polymorphic forms and the monohydrate of a nonsteroidal anti-inflammatory and analgesic drug piroxicam from acetone-water solutions have been investigated. Cooling crystallization of piroxicam has been conducted with different operation parameters, such as temperature, supersaturation, solvent composition. The effects of six different additives on the formation of the different solid forms have been investigated. An in -line probe of ATR FTIR (attenuated total reflection Fourier Transform Infrared) spectroscopy was used to collect spectra during the nucleation of piroxicam, and the spectra were analyzed with multivariate data analysis methods to follow the concentration profile of piroxicam in the solution. Furthermore, the in-line collected spectra have been used to gain insight into the formation of nuclei under different operation conditions as well as the intermolecular interaction of the additives and piroxicam. It has been observed that the formation of the polymorphs and the monohydrate strongly dependent on the concentration of the solute, temperature, solvent composition and the presence of additives. The formation of the nuclei led to certain difference on the IR spectra, which suggested that IR spectroscopy can be used to probe the formation of the molecules aggregates that are formed before the nucleation, and thus to build up a feed-back control for the formation of different solid forms. Results obtained in the present work suggested a great potential of using ATR FTIR to study the nucleation mechanism of different solid forms, and furthermore the in-line collected spectra could provide valuable information regarding the complex intermolecular interactions between the solute, solvent, and additives. This molecular level knowledge will led to optimal design for the selective crystallization the desired solid form of APIs.

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

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Granulation is a key product design step in solid dosage manufacturing processes in the pharmaceutical industry. By using a combination of formulation and processing methods, the properties of the granules are modified and controlled. However, the granulation process is complex and therefore, despite having knowledge of all the variables during the process, precisely predicting the characteristics of the produced granules still remains a challenge. This leads to non-optimal unit operation and causes a significant failure rate during scale-up of the solid dosage manufacturing process to industrial scale. In this context, continuous twin-screw granulation has received increased attention as it can be embedded in a continuous manufacturing line which also includes dryer, product control hopper and tabletting machine making continuous powder to tablet production possible. A continuous process with 24/7 production capacity will eliminate scale-up requirements and intermediate storage. Moreover, the screws used in the granulator have a modular structure (interchangeable transport and kneading discs) allowing greater flexibility in equipment design. However, to cure the inefficiency issue, knowledge about continuous granulation should be further developed both under steady state and dynamic conditions. Application of mechanistic models that incorporate the understanding of the underlying mechanisms is therefore pursued. In this study, the principle constitutive mechanisms of a granulation system such as growth, aggregation and breakage are included in a population balance modelling framework. This was done for the different individual screw blocks of a continuous twin-screw granulator. The rate processes which are considered dominant in the kneading element regions of the granulator, i.e. aggregation and breakage, were included. Based on an experimentally determined inflow granule size distribution and mean residence time of the granulator, predictions of the outflow granule size distribution were made. The experimental data was used for calibrating the model for individual screw modules in the twin-screw granulator. This provided an improved insight into behaviour of the system. The results showed that the successive kneading blocks lead to a granulation regime-separation inside the twin-screw granulator. The first kneading block after wetting caused an increase in the aggregation rate, which was reduced after the second kneading block. Whereas, the breakage rate increased successively along the length of the granulator. Such a physical separation between the granulation regimes will be promising for future design and advanced control of the continuous granulation process.

[305]

Process-based Method for Reducing Product Losses in Pharmaceutical Manufacturing

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Pharmaceutical production processes are requested to become more cost effective without compromising the product quality. In this paper, we propose a method for reducing product losses, e.g., pre-flush of product solution, hardware dead volume or defective products. The primary target of the method is the manufacturing processes of sterile drug products, such as injectables, infusion solutions, or eye-drops. The method is structured with the following steps: (1) Analyze process flow, (2) Collect process data, (3) Characterize loss causes, (4) Generate improvement scenarios, and (5) Perform multiobjective evaluation. By performing these steps, superior scenarios can be developed, which are economically attractive, technically feasible and compliant to quality regulations known as Good Manufacturing Practice (GMP), out of other choices.

A couple of novel mechanisms are proposed to support execution of these steps. For example, categorization method of different loss causes is defined in order to help generating effective ideas in Step 3. Indicators for Step 5 cover the aspects of economy, technical feasibility and quality compliance, and multiobjective evaluation identifies Pareto-optimal and thus superior improvement scenarios to be further investigated.

Case study was performed on an industrial process. In Step 1 and 2, more than ten loss causes of two processes were analyzed, which were then characterized in Step 3. It was revealed that most of dominant losses are associated with the start and the end of a batch production, e.g., pre-flushing of filter unit. In Step 4, various ideas of technical changes were generated, and after mutiobjective evaluation, promising ones were selected. This case study demonstrated that the method can support developing superior scenarios of loss reduction, and thus the Plan-phase of the Plan-Do-Check-Act (PDCA) cycle of process improvement.

[382]

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

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Since large molecules are considered the key driver for growth of the pharmaceutical industry, the focus is shifting from small molecules to biopharmaceuticals. The list of approved biopharmaceutical drug products from the Food and Drug Administration (FDA) and European Medicines Agency (EMA) consists of approximately 50% freeze-dried products (Constantino and Pikal, 2004). Therefore, freeze-drying is the preferred way to stabilise biopharmaceutical drug products which are unstable in aqueous solution. However, freeze-drying requires a lot of energy and has a long processing time, making it a costly process (Burns, 2009; Gieseler, 2012). The largest fraction of freeze-dried biopharmaceutical products are therapeutic protein formulations and vaccines (Pikal, 2002).

Conventional pharmaceutical freeze-drying (lyophilisation) is a batch process that consists of three consecutive steps: freezing, primary drying (ice sublimation) and secondary drying (desorption of unfrozen water). During the primary drying step the temperature at the sublimation front is critical, and should not exceed a critical value (dependent on the freeze-dried product) to prevent cake collapse. In this project, the focus is on the modelling of the primary drying step. The purpose of the model is to use it to support future optimisation of the process parameters during operation of the freeze-dryer in a dynamic way. During primary drying only two process parameters are adaptable, i.e. the shelf temperature and the chamber pressure. In conventional pharmaceutical manufacturing, both process parameters are fixed, resulting in a conservative cycle. However, by dynamically updating both variables (i.e. resulting in a time variant Design Space), a substantial decrease in processing time can be obtained.

The modelling approach can benefit from incorporating model parameter uncertainty to prevent that the critical temperature at the sublimation front is exceeded. Once the time variant Design Space is created for a certain set-up (i.e. a combination of a specific product and a piece of freeze-drying equipment), the values for both process variables can be fed to the equipment and a significant decrease in processing time can be obtained. As a result, the cost of processing will also be decreasing. Moreover, end product quality is guaranteed.

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[405]

Plant-wide control of a continuous tablet manufacturing for Quality-by-Design based pharmaceutical manufacturing

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The pharmaceutical industry is strictly regulated, where precise control of the end product quality is necessary to ensure the efficiency of the drug products. In this work, a combined feed-forward/feedback (FF/FB) control system has been developed for a direct compaction continuous tablet manufacturing pilot-plant. The feed-forward controller takes into account the effect of process disturbances and raw material variability proactively while the feedback control system ensures the end product quality consistently. The feed-forward control loop is based on real time monitoring of the powder bulk density while the feedback control loops are based on the powder level of instrumented hopper, drug concentration, tablet weight and hardness. Powder blend density has significant effects on the end product quality of the pharmaceutical tablets and therefore has been selected as the feed-forward variable. The coupled FF/FB control system ensures minimum variability in the final product quality irrespective of process and raw material variations.

[430]

Systematic Retrofitting Methodology for Recrystallization of Thermally Unstable Active Pharmaceutical Ingredients

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Pharmaceutical production processes are gaining research attentions in the field of CAPE/PSE. In this work, we present a systematic method for retrofitting pharmaceutical manufacturing plants, together with an industrial case study.

The method consists of five tasks: (I) collection of process understanding/data, (II) creation of process model, (III) adaptation of the model for optimization, (IV) optimization and (V) interpretation. In Task I, an overview of the process is obtained by performing Path Flow Decomposition (PFD), which determines the sources and sinks of the all substance in a batch, and thus facilitates the creation of a model. In Task II descriptive mathematical models are created for every unit, which will then be validated with the measurement data of the plant. The aim of Task III is to transform the descriptive model into an analytical model, which relates the optimization variables to the objective function. In parallel to identifying variables to be optimized, analysis is performed on constraints, especially on the aspects related to the quality of the pharmaceutical products. All these information are considered in Task IV, i.e., optimization, where MINLP plays a central role. Task V runs simultaneously to all the other tasks, which resembles iterative nature of the design.

The methodology was applied to a manufacturing plant of a solid drug, where crude crystal is purified through the process of Dissolution-Filtration-Crystallization (DFC). In Task I, a trade-off was identified: the higher the process temperature, THH, the more degradation of the crude crystal; the lower the TH, the more amount of undissolved crystal. The process flow rate, F, affects also the overall yield. In Task II, process model was created with considering measured data, e.g. particle size distribution (PSD) during the dissolution for the heat exchanger. The descriptive model was adapted for optimization by incorporating accurate information, e.g., liquid-wall-liquid heat transfer. We were able to model reactive-dissolution of crystals with PSD inside the heat exchanger, which is the secondary novelty of the work. As Task IV, three alternative process layouts were considered. The insertion of coolers before and after the filtration unit enabled a substantial improvement, lowering the degradation reaction and thus increasing the yield of 5.5% and the net present value of 15.5%. The validity of the model was supported by the result of the performance of lab scale experiments on a plant with the same new layout. The experimental and the simulated result differed 1-2%.

The method is developed to be flexible and the application is not limited to the DFC processes. The methodology can show its weakness in case the data measurement is difficult, which may well occur in the pharmaceutical processes. In fact without experimental data neither the creation of empirical correlation nor the validation of the created model cannot be carried out. Although non validated models do not provide exact values, trends and behavior inside the plant can still be observed and discussed.

[645]

Sensitivity and Feasibility Analysis in Pharmaceutical Process Risk Assessment

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In the pharmaceutical industry, quality risk management (QRM) is an important aspect of process development. QRM focuses on ensuring patient safety by developing and implementing strategies to ensure consistent product quality. QRM involves identifying factors that can affect quality and developing control strategies to address these factors [1]. Often tools like failure modes and effects analysis (FMEA) are used to evaluate risk factors with respect to product quality. FMEA assigns a risk priority number (RPN) based on the severity, detectability and likelihood of occurrence for each potential failure mode identified. One shortcoming of FMEA is that the assignment of severity, occurrence and detectability values is based on expert opinion. Recently the case has been made for an increasing role of quantitative methods in risk assessment for chemical process systems [2]. This is due to issues with the subjectivity of expert-opinion approaches like FMEA, which tend to under estimate risk and fail to adequately account for process uncertainty [3].

Sensitivity analysis, a process of attributing variability in outcomes to sources of uncertainty, can make risk assessment more quantitative in nature. Sensitivity metrics can be used to rank factors with respect to their influence on product quality and thereby identify potential critical process parameters [4]. In risk assessment, sensitivity analysis can be used to rank failure modes with respect to severity or probability. In addition, feasibility analysis can be conducted on a process to identify its design space with respect to uncertain parameters. Feasibility analysis involves identifying the space within which a process remains operable given certain constraints on the system [5]. In the case of pharmaceutical processes, these constraints may be bounds on quality attributes. In this way, feasibility analysis can provide enhanced understanding of process robustness with respect to sources of variability.

This work will discuss the role of sensitivity and feasibility analysis in pharmaceutical quality risk management. Several methods for sensitivity analysis will be described and demonstrated using a case study based on continuous pharmaceutical manufacturing. In addition, surrogate-based methods for feasibility analysis will be presented. These will be applied to a pharmaceutical unit operation, and the results will be presented in the context of identifying design space for the process.

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[672]

Modelling of Crystallization of Solid Oral Drug Forms in a Dropwise Additive Manufacturing System

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Traditionally, the pharmaceutical industry uses batch processes to manufacture pharmaceutical products, which provide significant challenges for the industry. In recent years, US Food and Drug Administration introduced the Quality by Design approach and Process Analytical Technology guidance to encourage innovation and efficiency in pharmaceutical development, manufacturing and quality assurance. As part of this renewed emphasis on improvement of manufacturing, the pharmaceutical industry has begun to develop more efficient production processes with frequent use of on-line measurement and sensing, real time quality control and process control tools.

Under the US National Science Foundation supported Engineering Research Center for Structured Organic Particulate Systems (NSF ERC-SOPS), a dropwise additive manufacturing process for solid oral drug production has been developed as an alternative to conventional pharmaceutical manufacturing methods (Hirshfield, et al., 2014). This mini manufacturing process for the production of pharmaceuticals utilizes drop on demand printing technology for automated and controlled deposition of hot-melt based drug formulations onto edible substrates. The dropwise additive manufacturing system consists of a precision positive displacement pump, xy-staging, a hot air based heating system, online imaging and sensing, and temperature, pump and stage controllers. A supervisory control system, including on-line monitoring, automation and closed-loop control, is implemented on the process, in order to produce individual dosage forms with the desired dosage amount and crystal morphology (Içten, et al., 2014).

Product morphology depends on the crystallization temperature; therefore the drop solidification process following the drop deposition on the substrate should be controlled (Nagy and Braatz, 2012). This is achieved indirectly by manipulating the substrate temperature profile using controlled temperature gradients. The solidification and crystallization processes of the drug deposits will be modeled using temperature dependent crystallization kinetics and cooling profiles monitored via the spectroscopic techniques, such as Raman, and IR camera. For the model formulation, the solid state transformation of the drug in the presence of polymer will be modeled to investigate the stability of the dosage forms. Using the proposed model, the temperature profiles leading to the desired solid state can be optimized.

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[720]

Model based control of recombinant E. coli fed-batch fermentation processes – implementation and evaluation of feedback control regimes

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In the course of the implementation of FDA`s Quality by Design approach advanced process monitoring, multivariate data analysis, modelling and model predictive control are the key tools. The fermentation process with living cell employed as production machineries is the most complex part in the processing chain of biopharmaceuticals and consequently full understanding of the cellular system, the process and the product are hard to achieve.

In this work a recombinant E. coli fermentation process was characterized in detail with special focus on how induction strength, temperature and growth rate influence product quality and yield. These process variables were varied within defined ranges and a comprehensive off- and on-line process data set was generated and then analyzed via multivariate statistics. The outcomes of this work were predictive models for cell dry mass, soluble and insoluble product with high prediction performance and a detailed process understanding.

Provided with this information a processing strategy aiming at a constant induction level defined via the inducer to biomass ratio was developed. The real time information on the actual cell dry mass in the system required for design of the feedback control loop was delivered by a radial basis function artificial neuronal network (RBF-ANN). The required real-time data preprocessing steps and RBF-ANN calculations were implemented via C# programming language by using the EVON process control software environment.

Functionality of the concept was shown with three process settings within the defined design space but unequal to process conditions used for model generation. With this setting we were able to keep the induction level constant throughout the process and to compensate for the decreasing glucose yield coefficient triggered by high recombinant protein production rates. Beside the proof of concept for model predictive control of fermentation processes the thus generated process data gave new insight into interdependencies between induction strength and product yield and open up space for more detailed analysis and process understanding.

[768]

Macroporous microparticles for pharmaceutical and medical applications

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The study presents several different ways of production of macroporous particles suitable for pharmaceutical and medical applications. Microparticles prepared are based on biodegradable chemical polymers and biologically active substances of protein nature.

In medicine such particles can be applied as material for implants and surgery, as sorbents for viruses and protein purification, as fillers for cosmetology, plates and matrixes for cell growth and may have other applications as well. They can be used in pharmaceutical industry as components of drug delivery systems, as a base for inhalable and nasal products.

Produced particles were investigated by SEM, residual moisture measurement, evaluation of pore size distribution, swelling properties study, adsorption study. The particles characteristics are as follows: spherical form, mean particle diameters are 0.2 – 1 mm depending on the production method, total porousity is up to 95%, residual moisture content 3-6%, pore network is rich, that predefines high swelling (1200%) and adsorption properties, comparable with widespread natural sorbents.

The production process was developed and piloted at laboratory scale, it includes dispergation into cryogenic liquid by means of a nozzle, particle structure formation at negative temperatures, followed by freeze drying (either under vacuum or at normal pressure conditions).

Potential medical and pharmaceutical applications of produced particles have been examined, initiating first preclinical trails and next steps of the technology and product development.

[813]

Optimal Resin Selection for Integrated Chromatographic Separations in High-Throughput Screening

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In the biopharmaceutical industry, high-throughput screening (HTS) allows for the rapid exploration of larger design spaces, and is applied in process characterisation for molecules in preclinical, clinical, and commercial manufacturing processes. HTS is widely used in the chromatography development. At the early stage of the drug development, different resins are tested under various operating conditions by implementing microscale experimentations on a robotic platform. When there are many resins for testing, huge amounts of data are generated. However, when faced with such extensive experiment data, the question that arises as is how to determine the optimal separation resins and conditions. Thus, systemic approaches for resin selection are required to facilitate the decision-making process, and prevent it from becoming a bottleneck.

We developed an optimisation-based approach to process high throughput screening data generated from microscale experiments and to identify the best resins in terms of target protein yield and purity. A novel optimisation framework, based on mixed integer linear programming (MILP) techniques, was developed, for optimal resin selection for a protein purification chromatographic sequence. An MILP model was firstly developed for a single-step separation. Then, the developed model was extended to cover a two-step chromatographic separation.

The developed optimisation models were applied to an industrial-relevant example with cation exchange (CEX) and mixed mode (MM) chromatography steps. When two chromatographic steps were optimised simultaneously by the proposed model, the solutions proved to be better than those from the optimisation of the two steps separately. The computational results show that the developed approach is an efficient way to identify the best resins for a two-step separation, with the benefit of saving time and reducing downstream processing costs at the early stages of drug development.

[931]

Plantwide design and economic evaluation of two Continuous Pharmaceutical Manufacturing (CPM) cases: Ibuprofen and Artemisinin

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Continuous Pharmaceutical Manufacturing (CPM) is a rapidly expanding research field with growing industrial importance: challenging the current batch production paradigm, it has a documented potential to deliver key cost, efficiency and environmental benefits. Ibuprofen, the potent painkiller, and artemisinin, a highly effective anti-malarial drug, have been identified as promising CPM candidates, and steady-state flowsheet models have been developed on the basis of published continuous organic synthesis pathways. Reactor design has been conducted using original kinetic parameter estimation results. A comparative economic analysis via published recoveries has computed performance indices which indicate that both CPM designs exhibit high economic potential, even if conservative profit and climate estimates are used to derive capital and operating costs. More detailed technoeconomic analyses can facilitate quicker CPM implementations.

Track 9.4. Food Systems Engineering

[303]

Data-based multivariate modeling of a grain comminution process

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The grinding of wheat into flour is one of the mankind's most ancient industrial processes [1]. The aim of wheat milling is to break open the kernel and to separate its structural components (endosperm, bran and germ) in such a way as to recover endosperm in maximum quantity at minimum contamination (with bran and germ), and at minimum cost. To achieve this objective, a gradual reduction approach is used through repeated milling and sifting unit operations. This configuration greatly increases the yield of flour than can be achieved, but makes the process more difficult to monitor and control.

The issue is exacerbated by the natural origin of wheat, which, as a natural product, exhibits a high intrinsic variability affecting the overall process significantly. Therefore, the millers' main challenge is to produce flour of consistent uniform quality, in the face of a constantly changing feedstock. Nowadays the control over the process is mostly based on the operators' experience, also due to the lack of instrumentation in industrial plants.

In view of the above, there is a great interest in finding systematic approaches that can support the operation of the process, for example by predicting the product quality profile, or that can be exploited to optimize the process operating conditions. Only a few main processing parameters influence the milling operation. Clearly the first goal is to understand and quantify the correlation between these parameters and the product quality.

In this study we exploit latent variable techniques (namely, principal component analysis [2] and partial least-squares regression [3]) to build data-based multivariate models that link process parameters and wheat properties to the final product quality. It is shown how the use of models in their "direct" form allows to improve process understanding and to predict the product quality profile. Furthermore, it is verified that, by inverting the data-based models, it is possible to determine the optimal combination of process parameters and wheat properties leading to a desired product quality.

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[734]

A comprehensive sensitivity and uncertainty analysis of a milk drying process

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A simple steady state model of a milk drying process was built to help process understanding. It involves a spray chamber and also internal/external fluid beds. The model was subjected to a statistical analysis for quality assurance using sensitivity analysis (SA) of inputs/parameters, identifiability analysis (IA) of parameters, and uncertainty analysis (UA) to estimate confidence intervals on parameters and in model predictions. A local method was used for SA, IA was based in the delta mean square and collinearity index calculation, and Maximum Likelihood Estimation was used as the main UA technique. SA results provide evidence towards over-parameterization in the model, and the chamber inlet dry bulb air temperature was the variable (input) with the highest sensitivity. IA results indicated that at most 4 parameters are identifiable: two from spray chamber and one from each fluid bed dryer. Moreover, the confidence intervals obtained for identifiable parameters were reasonable, although two parameters were found significantly correlated. The obtained confidence intervals for model predictions reflect a low uncertainty for the outputs. The rigorously analyzed model is expected to contribute to model-based decision making for process operation and optimization.

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[876]

Optimization of Production Planning and Scheduling in the Ice Cream Industry

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Throughout the years, the food industry has been growing. This growth has been driven by the increase of new market competitors, as well as, consumers' demands increase and exigency. These factors combined have changed the trends in such industry and a need for production optimization is a current need.

As part of the food industry, the ice-cream industry faces similar problems when considering the production scheduling, where one of the major problems is the perishable phenomena, which should be considered simultaneously with other operational aspects. The perishable phenomena offers special challenges as it affects production from the raw materials till the final products. This is reflected in the products freshness, aspect most sensible for the customer. Consequently, the inventory management of the raw materials and the product shelf-life are to be addressed so as to maximize the period between the final products production and the costumer consumption. Additionally, to the perishable characteristics another main aspect that needs be addressed when scheduling production within the food industry is the changeovers. Changeovers involve equipment washing, man-power allocation as well as any equipment set-up. The minimization of the associated times is also a goal to be considered so as to improve production, time and costs.

The problem described requires mathematical programming models where the batch process involving equipment resources shared by multi-task, and multi product should be modelled. To meet this challenge this paper presents a Mixed Integer Linear Programming (MILP) model based in the RTN representation. The characteristics of the ice cream industry are explored in detail where perishability, changeover times and multiple deliveries as well as other features of such industry are accounted for. The solution of a real ice-cream production in a Portuguese industry is performed.

Track 9.5. Energy Systems Engineering

[23]

Evaluation of Energy Integration Aspects for Advanced Chemical Looping Systems Applied for Energy Vectors Poly-generation

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Finding energy efficient and economic ways to convert fossil fuels and renewable energy sources to electricity or other total or partial decarbonised energy vectors (e.g. hydrogen, heat, synthetic fuels, methanol, DME etc.) is of paramount importance in modern society. The development and deployment of carbon capture, utilisation and storage (CCUS) technologies is equally important for transition to low carbon economy. This paper evaluates various energy vectors poly-generation (focusing on power, hydrogen and synthetic fuels production) based on chemical looping systems with total or partial decarbonisation of the used fuel. As illustrative examples, iron and calcium-based chemical looping systems were assessed in various plant configurations to generate total or partial decarbonised energy vectors e.g. plant designs with about 400 MW net power having a flexible hydrogen output in the range of 0 to 200 MWth (LHV) or 500 MWth substitute natural gas (SNG). The products flexibility (the capability of evaluated plants to change the generated energy vectors according to the timely demand from the grid) is an important aspect in modern energy conversion systems. The carbon capture rate of evaluated energy conversion concepts is almost total (>95%). In addition, considering biomass (e.g. sawdust, agricultural wastes) or other solid wastes (e.g. municipal solid waste, sewage sludge) co-processing, the investigated concepts have negative fossil CO2 emissions.

The paper presents in details evaluated plant configurations, focusing especially on operational and mass & energy integration aspects. The designs were modelled and simulated using process flow modelling software, the results being used to assess the overall performance indicators (e.g. energy efficient, ancillary power and water consumption, fuel usage, specific CO2 emissions etc.). For energy integration analysis, pinch method was used to evaluate and find the best energy integration options of available heat generated in the chemical looping cycle into overall steam cycle of the power block. Other mass and energy integration aspects, e.g. air integration between the air separation unit and the gas turbine, plant flexibility in terms of changing generated energy vectors vs. time, were evaluated as well to assess their influence on overall plant energy efficiency. For comparison reasons, benchmark cases were considered, e.g. gasification-based energy conversion scheme with carbon capture based on gas-liquid absorption (using physical and chemical solvents). As the results show, the chemical looping configurations for energy vectors poly-generation have significant advantages compared to other more technological and commercial mature carbon capture options (e.g. gas-liquid absorption), the more important being the higher energy efficiency and carbon capture rate, reduced capital and operational costs, ability to process higher ratios of biomass (a significant issue for conventional gasification processes), lower (or even zero) oxygen consumption, lower plant complexity etc.

[156]

Synthesis of Biomass-based Trigeneration Systems with Reliability Aspects

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Trigeneration systems are utility systems which produce heat, power and cooling simultaneously from a single fuel source. With such efficient use of fuel, installing trigeneration systems on-site would be beneficial as it reduces the importation of power and fuel, reduces emissions, and improves local power reliability. In order to realize these benefits, trigeneration systems are required to have a reliable network of component process units, since the high level of integration increases the likelihood of cascading failures. Each unit may not always be available to function because it may require preventive or corrective (e.g. when the system fails) maintenance during the course of operations. Traditionally, this issue is handled by installing additional process units based on rules of thumb or heuristics. The use of heuristics however, may not be able to address complex decisions on whether to purchase a single unit with larger capacity or multiple smaller capacity units offering a degree of redundancy. If not addressed appropriately, such decisions may result in excessive capital and maintenance costs. In addition, the design may not be able to fulfil specified demand requirements, especially under seasonal variations. To address these issues, this work presents a systematic procedure for synthesizing a trigeneration system considering equipment redundancy based on reliability theory. To illustrate the proposed approach, a simple case study on synthesizing a steam turbine configuration for a biomass-based trigeneration system (BTS) is presented.

[180]

Optimization of the cost of compression in the Finnish natural gas pipeline

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In Finland natural gas is today distributed to the southern parts of the country with a pipeline from Russia. The gas is mainly used for electricity and heat production. In 2012 about 33.2 TWh of natural gas was delivered to the customers in Finland. The extension of the distribution pipeline network to other cities is being considered. Further possibilities to provide the Finnish customers with natural gas are to connect regasification facilities from liquid natural gas (LNG) terminals or sites with biogas production to the pipeline. The construction of LNG terminals and storages is seen a means to increase the independence of Finland on the energy deliveries while the use of biogas will lower the emissions considerably.

The ambient temperature strongly influences the demand of heat and electricity in Finland. In order to study a potential expansion of the gas distribution network and the use of new gas sources, the present natural gas system was modelled and simulated on a daily basis for a reference year, considering the main consumers and the seasonal variations in the energy demand. This gave the gas flow rates and pressures in the pipes, as well as compressor duties for every day. The possibilities to extend the pipeline to other cities was studied, and the implications for the additional supply on the system was analysed, revealing extra need of compression and the feasibility of the system at these new states. The expansion problem was stated and solved as an optimization problem, yielding information about an optimal design of the new parts of the network and the locations of possible compression units. Finally, an attempt was made to optimize the integration of an LNG terminal from which regasified natural gas was supplied to the pipeline.

[194]

Multi-Objective Optimization of Heat Exchanger Network Retrofitting Considering Variable Heat Capacity and Structural Modifications

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Heat exchanger networks (HEN) are employed in process industries to decrease external utilities consumption and for economic and environmental sustainability. Retrofitting existing HEN can achieve significant energy savings for a relatively small investment. It is useful for numerous plants designed in the past and operating currently. Mathematical programming methods are increasingly used to solve HEN retrofitting problems. Of these, stochastic global optimization (SGO) methods such as genetic algorithms and differential evolution are gaining popularity. These methods have been applied to HEN retrofitting problems having constant heat capacity and/or for single objective optimization [1]. This study considers variable heat capacity and multi-objective optimization (MOO) as well as different levels of HEN retrofitting. The objectives used in MOO can be investment cost, utility cost, total annualized cost, number of reassignments and number of heat transfer enhancements.

Retrofitting can be performed at various levels: modifying the HEN structure which includes adding new heat exchangers, additional area in existing heat exchangers and re-sequencing the existing matches (including re-piping, reassigning), and/or using heat transfer enhancements. This work investigates systematically HEN retrofitting at different levels from relatively easy to more difficult for implementation. For this, MOO is applied to different levels of retrofitting the HEN of a crude distillation unit [2], having 10 hot and 3 cold streams with varying heat capacities; the existing network has 18 exchangers including 3 heaters and 9 coolers. The objectives used are investment for retrofitting, utility cost after retrofitting and extent of heat transfer enhancement used. MOO is performed using the elitist non-dominated sorting genetic algorithm (NSGA-II) for different levels of retrofitting. Thus, there will be one Pareto-optimal front for each of the levels. An optimal solution can be chosen from one of these fronts based on the scenario in the plant (e.g., budget, manpower and time available for retrofitting). The optimal results generated by MOO of retrofitting the HEN of the crude distillation unit will be presented and discussed at the PSE 2015.

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[195]

Operation and control of concentrated solar power plant with energy storage system

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Concentrated solar power (CSP) is one of potential technologies to harness solar irradiation into thermal and electrical energy. Generally, CSP system consists of three subsystems including a solar collector, a thermal storage and a power cycle. The principle of this technology is to concentrate the solar irradiation by a set of mirrors in the solar collector to produce high temperature heat. The heat received is then absorbed by a working fluid and transported to the storage or a boiler where steam is produced. The steam produced is then used in the power cycle to generate electrical power.

CSP system is environmentally friendly and not contributing to the rising amount of greenhouse gases or other pollutions. Moreover, It also provides advantages over photovoltaic (PV) system. It has the capability to efficiently storage energy in a form of heat. The stored heat can be either converted to electricity or directly used in a form of heat, which is far more efficient than in a form of electricity. Moreover, CSP system uses a conventional process to generate the electricity resulting in alternate current (AC) electricity. In comparison, PV system produces direct current (DC) electricity. The DC electricity produced is then converted into AC electricity.

Solar energy is of unsteady nature, and the disturbances strongly influence the system performance. In this work, a dynamic model of CSP system consisting of a central receiver, a two-tank thermal storage, and a Rankine cycle was developed using a commercial simulator, Dynsim. The model developed was validated against literature data, and the results showed good agreement. The dynamic simulation was performed in a number of case studies, and control scheme was proposed. The control performances of the system were analyzed. The control scheme proposed can effectively stabilize the system.

[205]

Optimal integration of the year-round operation for methane production from CO2 and water using wind, solar and biomass

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Most of the sustainable sources of energy, namely biomass, wind and solar, present variable availability with time, seasonality, day-long variability, and region, which results in the fact that storage systems, supplementary sources of energy or a combination of some of them (Yuand and Chen, 2012) are needed to maintain the production capacity and to meet the demand.

In this paper we integrate the use of lignocellulosic biomass, wind and solar energy for the constant production of synthetic methane over a yearlong as a means to store energy as a ready to use fuel. The biomass is used to produce syngas considering direct or indirect gasification followed by steam reforming or partial oxidation to remove the hydrocarbons. The clean syngas can be used to produce electricity in a Brayton cycle, or hydrogen using the water gas shift reaction. On the other hand, photovoltaic solar and/or wind energy are used to obtain power which, alone or together with that generated from the biomass, is used for water electrolysis to generate hydrogen and oxygen. While the oxygen is stored, the hydrogen is used to synthesize methane with CO2 from flue gases. We formulate the problem as an MINLP to optimize the topology of biomass processing and we select the best combination of technologies. Next, we perform a sensitivity analysis to evaluate the limiting conditions for the use of the different resources.

For current prices and in a particular location with high wind velocity and solar incidence, Cádiz (Spain), the biomass is processed via indirect gasification and steam reforming followed by the Brayton cycle to produce electricity. The biomass based electricity tops that obtained using PV solar. Hydrogen is produced from water electrolysis and not from the biomass. The investment cost is of 175 M€, and the production cost is of 0.38€/Nm3 of methane. Next, a sensitive analysis is performed to evaluate the effect of solar and wind availability and the biomass price level at which either of the renewable sources is preferred. The use of biomass is recommended for a raw material price below 50€/t and investment rates below 1500€/kW. Wind and solar complement the biomass, and only when biomass processing is too high, solar is used as long as its incidence is above 1200 kWh/m2 yr. The use of wind is recommended for regions with low solar incidence and wind velocities above 9 m/s.

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[207]

Optimal Scheduling of Air Separation with Cryogenic Energy Storage

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The concept of cryogenic energy storage (CES) is to store energy in the form of liquid gas and release it when needed by evaporating the gas to drive a turbine. The CES technology is being pioneered in the UK (Harrabin, 2012) where the company Highview Power Storage has been running a liquid air energy storage (LAES) pilot plant since 2011.

Although CES on an industrial scale is a relatively new approach, the technology is well-known and essentially part of any air separation unit (ASU) that utilizes cryogenic separation. In this work, we assess the operational benefits of adding CES to an existing air separation plant. We investigate three potential new opportunities for an integrated ASU-CES plant: (1) increasing the plant's flexibility for load shifting, (2) storing purchased energy and selling it back to the market during higher-price periods, (3) creating additional revenue by providing operating reserve capacity, which is required when the real-time electricity demand in the power grid is higher than the supply, e.g. due to unexpected load increase or generator failures.

We develop a mixed-integer linear programming (MILP) scheduling model for an ASU-CES plant, which is based on a formulation proposed by Mitra et al. (2012). Furthermore, to model the uncertainty in reserve demand, we apply a robust optimization approach (Bertsimas & Sim, 2004) that allows control over the level of conservatism.

The proposed model is applied to an industrial case study provided by Praxair. The results exhibit typical relative cost savings of approximately 10% under relatively conservative CES efficiency and uncertainty assumptions. Especially for an air separation plant that has to satisfy gas as well as liquid demand, using CES leads to significant reduction in gas that has to be vented and therefore wasted due to overproduction. A sensitivity analysis shows that besides the CES efficiency, economic benefits strongly depend on the level of plant utilization. If the level of utilization is low, which allows high flexibility for load shifting, cost savings can be even considerably higher. This suggests that an added CES system may be an especially good option for underutilized air separation plants.

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[297]

Economic Optimization of Biorefineries

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Second generation biorefineries reached commercial reality in 2012 leading to the first commission of a large scale plant in October 2013 by Beta Renewables in Crescentino, Italy. Second generation biorefineries transform lignocellulosic agricultural wastes into products with higher added value. In biorefineries employing biochemical routes, this is achieved by the following four major conversion and separation technologies: biomass pretreatment, enzymatic hydrolysis, fermentation and purification. Lignocellulosic biomass consists of cellulose, hemicellulose (xylan and arabinan), lignin, ash and other residues in negligible amount. Cellulose is protected by layers of hemicellulose and lignin, and the scope of the pretreatment phase is to expose the cellulosic fibers by relocating lignin and partially hydrolyzing the hemicellulose. Hemicellulose should only be partially hydrolyzed because most of the pretreatment by-products inhibit the downstream processes. For example, acetic acid influences the pH of medium, which affects the enzymatic activity, furfural is a fermentation inhibitor, and xylose and xylooligomers strongly inhibit the enzymatic activity in the liquefaction phase. Therefore there is a trade-off between biomass pretreatment and the efficiency of the subsequent enzymatic hydrolysis and fermentation processes.

In the liquefaction phase, also known as the enzymatic hydrolysis phase, enzymes hydrolyze both cellulosic and the remaining hemicellulosic fibers. The conversion route of fibers to sugars is usually considered to be a competitive product inhibition thoroughly described and analyzed. Xylose and xylooligomers are the strongest inhibitors of liquefaction, even greater than cellobiose and glucose. Too little biomass pretreatment would increase the amount of hemicellulose for liquefaction, which would eventually decrease the glucose yield due to xylose and xylooligomers inhibition. On the other hand, too much biomass pretreatment would increase the amount of acetic acid and furfural. A great amount of pretreatment would be beneficial for liquefaction but not for fermentation.

The first scope of this study is to formulate optimal operation of commercial scale biorefineries as a mathematical programming problem. In this formulation, the performance trade-offs between pretreatment, liquefaction and fermentation is formulated as objective functions subject to system dynamics taking into account the above mentioned phenomena using previously developed and validated first principles dynamic models. For example, too much xylan in the liquefaction phase could be overcome by significantly increasing the enzyme dosage. However, enzymes are very expensive and operation costs would increase. Therefore, price tags need to be attached to raw materials, such as: raw biomass, steam for pretreatment, enzymes for liquefaction, and base for pH adjustment both in liquefaction and fermentation phase. The second goal of this study is to extend the formulated performance trade-offs with economic factors for all raw materials. The final outcome would be to use the cost functions in order to find the best possible trade-off between the optimal operation of pretreatment, liquefaction and fermentation processes in integrated manner. The optimization study will be applied to a commercial scale second generation biorefinery data.

[324]

An Integrated Unit Commitment and Generation Expansion Planning Model

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For decades, traditional long-term generation expansion planning models are based on simplifications with regard to operational costs and issues ignoring technical details such as start-up and shut-down related decisions, ramp rates and operating reserves. This approach has been successfully implemented on the grounds that load profile was highly predictable and with quite slow time dynamics. However, due to the intermittency and high fluctuations of rapidly penetrated renewable energy technologies (e.g., wind and solar), the net load required to be covered by the traditional hydrothermal power plants is characterized by higher uncertainty and has faster time dynamics. As a result, it is highly debatable how much operational detail has to be introduced into the long-term planning models in order to adequately secure the validity and the robustness of the investment decisions to be implemented. For these reasons, the incorporation of short-term decisions (unit commitment problem) into the long-term planning framework (generation expansion planning problem) is able to enhance and strengthen the accuracy of the decisions to be made and guarantees the stability of power networks.

This work presents a generic mixed integer linear programming (MILP) model that integrates the unit commitment problem (daily energy planning) with the long-term generation expansion planning framework. Typical daily constraints at an hourly level such as start-up and shut-down related decisions (minimum up and down time, synchronization, soak and desynchronization time constraints), ramping limits, system reserves requirements are combined with representative yearly constraints such as power capacity additions, power generation bounds of each unit, peak reserve requirements, and energy policy issues (renewables penetration limits, CO2 emission cap). For modelling purposes, a representative day (24 hours) of each month over a number of years has been employed in order to determine the optimal capacity additions, electricity market clearing prices, and daily operational planning of the studied power system. The model has been tested on an illustrative case study of the Greek power system. Our approach aims to provide useful insight into the strategic and challenging decisions to be determined by investors and/or policy makers at a national and/or regional level by providing the optimal energy roadmap according to specific assumptions and projections (electricity demand, fuel prices, and investment costs).

[331]

System Design of Renewable Energy Generation and Storage Alternatives for Large Scale Continuous Processes

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The use of renewable resources as an alternative for energy generation has been widely researched. However, the intermittent, seasonal and often unpredictable nature of renewable resources has been a major concern, limiting its use in industrial-scale processes. As such, the development of suitable energy storage alternatives is an important challenge that must be overcome if such processes are to be operated off-grid. This is particularly important for continuous processes such as mining, where variations in process energy demands often exist. This work presents a system model for the economic evaluation of storage alternatives, thereby providing a bridge between energy generation and supply for such processes. It also investigates the behaviours of the storage alternatives to energy demand and supply variations by considering the demands of a remotely located mine in Chile.

The model presented in this work determines the optimum combination of storage alternatives for the supply of heat and electricity to meet the varying demands of the process with the available solar resource based on the minimization of the capital cost. A superstructure model combining three storage alternatives is developed in this work: Pumped Hydraulic Energy Storage (PHES); Advanced Adiabatic Compressed Air Storage (AA-CAES); and molten salt two-tank storage. For PHES, a plant with a reservoir height difference of 1000m, which stores energy generated from PV, is modelled. The AA-CAES also receives energy from PV and comprises of two compressors and turbines. The air storage pressure is maintained constant at 50bar, with interstage cooling and heating incorporated. Reinforced concrete is selected for thermal energy storage [1]. For the two-tank salt system, the system modelled consists of a CSP plant with thermal salt stored in a two-tank system, similar to [2]. The methodology involves the ab initio development of the models for energy generation and storage, with material and energy balances generated for each of the storage alternatives, leading to the development of a mixed integer non-linear programming (MINLP) problem. Within the paper, the demands of the mine are considered as a case study to illustrate the techniques used.

With the developed model, a better understanding of the daily and seasonal behaviours of energy storage systems is gained. The effect of process demand variations on process behaviour may be studied. The model gives a better understanding of the non-linear nature of storage models. The model also gives an insight into the losses encountered in energy storage and the efficiencies of the selected storage options.

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[349]

Energy assessment of different configurations for the ethanol production process from lignocellulosic biomass

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The production of biofuels for energy generation from renewable sources is rapidly becoming a widely studied research area that aims to find new approaches and technologies with which biofuels can be obtained, not only efficiently, but profitably. This work considers the production of ethanol from corn stover, a lignocellulosic biomass. The production of ethanol from lignocellulosic biomass has been identified as a high energy-consuming process and its implementation in industry has therefore so far not been completely successful. The process consists of two sections: a fed-batch section which comprises the pretreatment, detoxification, enzymatic hydrolysis and fermentation, and a continuous section that may combine different separation methods such as distillation, adsorption and/or pervaporation. The continuous section usually accounts for the highest energy requirements.

This works simultaneously considers the optimal design of both the fed-batch section and the continuous section, as well as the optimal distribution of the heat requirements within the overall process. In particular, this work investigates three different arrangements of the continuous separation section. The first configuration comprises two distillation columns and a hydrophilic membrane system used to dehydrate ethanol beyond the azeotropic point. This arrangement is the traditional configuration used in the production of ethanol from biomass. The second configuration introduces an organophilic membrane system for the removal of ethanol from the fermentation broth, followed by a distillation column and a hydrophilic membrane system. The third approach additionally considers recycling the retentate stream from the organophilic membrane system back to the fermentation reactor to further the production of ethanol by re-processing the unreacted substrate. For each arrangement, the overall energy demand is evaluated in order to identify the required heat sources and to distribute these more efficiently within the process. The energy distribution is carried out by transferring the heat released, for instance, from the condenser of the distillation columns, from steam utilities and from process hot streams to other units such as heat exchangers so that the overall energy demand is minimised.

The results show that the inclusion of the organophilic membrane system following the fermentation reactor but prior to the distillation column reduces the overall energy consumption in the process significantly and also represents a reduction in the size of the plant. Recycling the retentate from the organophilic membrane system is also found to be an improvement for the overall process as the concentration of ethanol from the fermentation increases, and therefore the energy demand in the distillation column decreases.

[360]

An Industry View on Improving Energy Efficiency - Developed Methodologies, Applied Tools and Collected Experience

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In the last decade the significant reduction of the energy demand of manufacturing processes came into the focus of the process industry. Due to dramatically raising energy prices, stricter environmental protection regulations and additional costs on CO2 emissions the energy costs became a major share of the overall production costs. In this context, Bayer has committed itself to reduce the group-wide specific greenhouse gas emissions by 20% until 2020 based on the reference year 2012.

The submitted contribution will give an insight into the developed methodologies, applied tools and the collected experience.

For an efficient reduction of the greenhouse gas emissions a valid and consistent data set of the as-is state of the plant is necessary. Therefore, the methodology of the Bayer Energy Efficiency Check was developed and has been successfully applied to 150 plants worldwide so far. The daily tracking and monitoring of the energy demand is also essential. The developed energy efficiency management system STRUCTese® (Structured Efficiency System for Energy) provides to every point of time the full transparency of the actual operational state through a detailed energy loss cascade which assigns losses to different cause categories [1]. The methodology has been implemented in Bayer's most energy intensive production plants.

Further significant energy savings can be achieved by a holistic optimization of the whole manufacturing site. Such Total Site Analyses are economically beneficial but very challenging at the same time.

Having powerful methodologies and tools available does not ensure energy efficiency. The human factor is even more important. Each analysis, development and implementation step was done in close interaction with the customers' plant and operating staff. In this way, a mutual understanding of the different and partly conflicting targets was achieved. This enables the improvement of both, the energy efficiency of the plants and the previously described methodologies and tools for increasing the energy efficiency.

The economical and ideal success has changed the companies' view on the topic. Many targets have already been achieved. However, there are further challenges we are currently facing.

Acknowledgement

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[415]

A computer-aided scenario analysis of future energy demand/supply systems: A case study in Japan

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The design of energy systems has become an issue all over the world. A single optimal system cannot be suggested because the availability of infrastructure and resources and the acceptability of the system should be discussed locally, involving all related stakeholders in the energy system. In particular, researchers and engineers of technologies related to energy systems should be able to perform the forecasting and roadmapping of future energy systems and indicate quantitative results of scenario analyses. A computer-aided analysis is strongly needed for such purpose.

We developed an energy flow model developed for analysing scenarios of future energy systems implementing a variety of feasible technology options (Kikuchi, Y., et al. Applied Energy, 132 (2014) 586-601). The model was modularized and represented as functionals of appropriate technology options, which enables the aggregation and disaggregation of energy systems by defining functionals for single technologies, packages integrating multi-technologies, and mini-systems. In this study, we expanded and applied this model into the future energy-system design in Japan.

The combinations of technologies on both energy supply and demand sides can be addressed considering not only the societal scenarios such as resource prices, economic growth and population change but also the technical scenarios including the development and penetration of energy-related technologies such as distributed solid oxide fuel cells in residential sectors and new-generation vehicles, and the replacement and shift of current technologies such as heat pumps for air conditioning and centralized power generation. Hourly-daily power load curve was taken into account for the annual power-supply planning in 365 days for unstable power sources and supplemental technologies such as photovoltaic power and secondary batteries. Through case studies, it was demonstrated that the potential of energy technologies can be analysed by the developed model considering the mutual relationships of technologies. The contribution of technologies to, e.g., the reduction in greenhouse gas emissions should be carefully examined by quantitative analyses of interdependencies of the technology options.

[418]

Integrated Solar Thermal Hydrogen and Power Coproduction Process for Continuous Power Supply and Production of Chemicals

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Diminishing fossil fuel reserves and increasing atmospheric greenhouse gas (GHG) levels make essential the utilization of alternative renewable energy sources to meet energy needs. Development of renewable power production technologies is especially important since electric power is the largest consumer of primary energy resources and it has the highest growth rate among alternate energy use sectors. Additionally, electricity sector is currently responsible for greater than 40% of the global CO2 emissions.

Among the renewable energy sources, solar energy is prominent due to its abundance. Yet intermittencies and land availability constraints for solar energy collection are the grand challenges for solar thermal power generation and demand a high efficiency solar power generation cycle that synergistically integrates energy storage.

Here, we introduce a system analysis of the newly developed solar thermal power and chemical co-production process (SPCCP). The process produces and stores solar thermal power efficiently to enable round-the-clock power supply. SPCCP constitutes of three novel processes: (i) solar thermal power cycle [1], (ii) thermal chemical production process [2], and (iii) chemical combustion power cycle [2].

Solar thermal power cycle [1] has a potential to generate electricity with sun-to-electricity (STE) efficiencies greater than 30% at low solar heat collection temperature. The cycle also promises STE efficiencies greater than 45% for the high solar heat collection temperatures.

For the cases with higher solar heat collection temperatures, the solar thermal power cycle is integrated with the chemical production process to coproduce chemicals for storing energy from solar irradiation. When solar energy is not available, the produced chemical can be utilized using the novel chemical combustion power cycle to supply electricity continuously. The overall sun-to-electricity efficiency of a twenty-four hour cycle is estimated to be greater than 34%. In summary, we propose a thermodynamic cycle that has the potential to generate uninterrupted electricity for grid distribution around the clock at GWh levels. The chemical produced from the integrated process can also be used as a feedstock for production of other chemicals.

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[516]

Synthesis Optimal Design of Microalgae-based Biorefinery under Uncertainty

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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 under modelled uncertainties.

[523]

Effect of feed natural gas conditions on the performance of mixed refrigerant LNG process

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For many countries around the world, natural gas (NG) is recognized as an important energy source from economic and environmental perspectives in the least. The NG liquefaction process is at the heart of the natural gas supply chain however it is an energy intensive process. The design and operation of liquefied natural gas (LNG) plants has been receiving significant industrial and research attention driven by the significant demand for NG and the sheer scale of the NG market. Efficient design and operation of LNG plants requires optimal process responses to various factors including upstream feed NG well conditions.

Recently, we studied the impact of numerous key variables including mixed refrigerant composition on the performance of a LNG plant (Wang et al., 2013). Another critical issue is the fact that the composition and flowrate of extracted natural gas varies over the life of a production well. These variations affect the performance, production and product quality of LNG plant. This paper is focused on understanding, through sensitivity analysis, the effect of feed NG composition and flowrate on process performance and LNG product for a C3MR LNG process. Feed gas compositions with various component ratios of methane (CH4) and other hydrocarbons for the given flowrate of natural gas are tested. Simulation results show that a higher amount of heavier hydrocarbon than ethane (i.e. propane and butane) in NG if present will require more energy use especially n-butane (n-C4H10) while higher amount of ethane is found to require less energy consumption than propane and butane. In addition, up to 2% of nitrogen (N2) by mole fraction in NG results in an additional 1.03% of specific power consumption. Carbon dioxide (CO2) concentration up to 2% appeared to reduce energy consumption by 0.2%. Overall, this study through a presentation of a model-based sensitivity analyses highlights the significance of the effects imparted by the feed NG composition and flowrate on the LNG process.

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A Spatial Decomposition Procedure for Efficient Solution of Two-Dimensional Energy Distribution Problems

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One expected development in the energy sector is that structures of energy systems and networks will in many cases move towards a more distributed, decentralised structure, with multiple smaller power plants and energy supplier units providing the energy previously commonly supplied by a large centralised plant. If well planned, these distributed structures are anticipated to increase the efficiency, flexibility and security of energy systems. Many mathematical models have been formulated for aiding the design process and analysis of distributed energy systems such as district heating systems. A search for optimal structures and multi-period operational schemes of district heating networks consisting of supplier, consumer and storage nodes connected via pipelines can be formulated as a mixed-integer linear program and solved using standard algorithms, but as the problem sizes increase, the solution times become too long for practical use. For this reason, a procedure for decomposing such an optimization problem in order to reduce the required computational time is proposed. This procedure is based on dividing the geographical area of the energy system into separate sectors which are treated as nodes in a simplified network. During consecutive iterations, the amount of sectors, along with the detail level of the simplified network, is increased. Each iteration reduces the search space of the original problem, thus reducing the time needed for the solution. While reaching global optima cannot be guaranteed, examples are given where the procedure finds better solutions than standard algorithms could find within any reasonable time limits.

[568]

Computational Platform for Optimal Design of Biorefineries Using Energy and Mass Integration

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Biorefineries are stated as promising alternatives for production of sustainable biofuels and chemicals which can replace fossil derivate products. The benefits from the efficient use of biomass as raw material in novel processes are mainly related with greenhouse gases emissions reduction when compared with petrochemical products. As in conventional oil-driven plants, the diversification of products in biorefineries promotes the integral use of the carbon source, being the key for reducing environmental impact and cost. Industrial synergies with mass and energy recovery can help to improve economic competitiveness on these bio-based plants that may face the problem of oil prices fluctuation and the incipient carbon emissions market.

The large number of possible biorefineries technologies currently under development and the complexity of these systems with several waste streams make the conversion pathway selection and the plant design difficult challenges to be solved. Optimization techniques have been used for biorefineries pathways selection but normally ignore the problem of energy supply to the plant, considering mass but not energy needs and having simplified technologies process models.

This paper presents the development of a computational platform for biorefineries design that includes mathematical programming techniques with combined mass and energy integration of processes. This innovative approach can assess the whole conversion chain, from the feedstock production to the final disposal of non-recovered wastes and show the optimum solution for the plant design. Local context constraints can also be included for applied research considering costs and environmental impact estimations.

A biorefinery models database is built to provide detailed information about mass and energy streams in industrial plants, making possible not only for biomass conversion pathway selection in large scale but also the design of single plants, including several alternatives of waste streams and by-products valorisation.

[575]

A rolling horizon stochastic programming framework for the energy supply and demand management in microgrids

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The growing interest in the exploitation of renewable energy sources has led to an increasing use of microgrids. One of the main drawbacks associated to this management problem is the presence of uncertainty. The main sources of uncertainty in this area are associated to the availability and production capacity of renewable energy generation units as well as the energy demand variations.

This work proposes a discrete-time Mixed Integer Linear Programming formulation based on a combined rolling horizon and stochastic programming approach for the simultaneous management of energy supply and demand in microgrids. This approach considers the available energy generation technologies, and energy balance equations that describe energy flows, production, storage and consumption levels. This formulation uses a stochastic programming approach, which considers different scenarios associated to variations in the duration of the energy consumptions, to contemplate all possible scenarios related to the energy demand. However, the high complexity related the estimate the weather forecast with a high degree of precision makes unaffordable the consideration of all possible external scenarios. The proactive stochastic formulation is introduced into a rolling horizon approach, to update all uncertain input parameters. The suggested methodology considers the updated information about the current state of the system, the confidence on the power availability and demand forecasts and the energy demand profile.

This approach is tested in a case study that consists of several renewable energy generators and energy consumers under uncertainty related to weather conditions and to the nominal duration of the energy consumptions tasks. Another particular feature is that delays in the target starting time of consumption tasks are allowed and, in case of deviation from this target starting time, penalty costs are implied. The main decisions to be taken include the production required from each energy generator at each period of time and the specific time to execute an energy consumption task.

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[580]

Behaviour Assessment of a Fuel Cell - Battery System Using a Supervisory Control Methodology Empowered by a Hybrid Timed Automaton (HTA)

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This work explores the behaviour of an integrated fuel cell and battery system for vehicular applications under various conditions. The system consists of a lithium-ion battery stack, a Polymer Electrolyte Membrane (PEM) fuel cell and a programmable electronic DC load. Besides the main objective of the integrated system which is the fulfillment of the load demand, it is important to consider the optimal use of the available hydrogen, the protection of the battery's lifetime and the preservation of the fuel cell's operability. Therefore, it is necessary to supervise and control the operation of all subsystems by using an appropriate Energy Management Strategy (EMS). The purpose of an EMS for such systems is twofold, to supervise the status of each subsystem and to be able to adjust the operational modes. Furthermore, as this is a multi-source power system, an EMS that can incorporate hybrid decisions is required. For these reasons a Hybrid Timed Automaton (HTA) is designed and developed which is able to handle the dynamic and the discrete decisions while considering the constraints and the boundaries of each subsystem. In that context the EMS is realized by an automaton based structure while the system requirements are implemented through a propositional based logic that represents a set of operating rules. The interactions among the electronic and the electrochemical subsystems are considered by the HTA that switches between the operational modes and determines the set-points of the field-level control loops. This methodology is not system specific and can be generally applied to other applications as well, since its architecture relies on generic elements that represent each subsystem of the considered case study.

In order to explore the behaviour of the proposed system a set of operation scenarios are selected. These scenarios are based on predefined driving profiles described by time-varying curves of power demand in order to be used for the sensitivity analysis, the optimization problem and for the evaluation of the overall behaviour of the system. Each subsystem is modelled and a sensitivity analysis is performed that reveals the main parameters and variables that affect the response of the integrated system. Subsequently a deterministic optimization problem is formulated that defines the optimum values for the parameters derived from the sensitivity analysis. The objective of the optimization problem is to enhance the performance and fulfil the integrated system's objectives. The overall behaviour and response of the system is analysed using quantitative metrics such as the depth of discharge or the state of charge of the battery and the hydrogen utilization. The flexibility and effectiveness of the proposed supervisory methodology is presented and the assessment of the system's behaviour reveals its potential, explores the synergy among the various subsystems and demonstrates the response of the integrated system.

[635]

Downstream Process Design for an Efficient Acetone, Butanol and Ethanol Separation from ABE Fermentation Broth

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The production of biofuels and high value-added products from lignocellulosic biomass, has gained special interest due to the possible reduction of crude oil production and the subsequent price increment of its derivatives in the market, lower greenhouse effects in the environment, etc. Among the different products from lignocellulosic material, butanol has been identified as a potential biofuel since it shows diverse advantages compared to other biofuel such as bioethanol. The production of butanol by a biotechnological pathway has been performed employing bacteria from the genera Clostridia. However, this manner also produce acetone and ethanol that might be a disadvantage because it would increase the complexity in the purification of butanol. There are several studies employing different separation technologies trying to overcome this issue, for example, heteroazeotropic distillation,[1] hybrid extraction-distillation process,[2] pervaporation and adsorption technologies,[3] etc. Most of the previous works has considered a hypothetical mixture using the main compounds of the fermentation broth (such as, acetone, butanol, ethanol and water), which can be a close approximation to the real mixture, but the presence of other compounds (e.g. not reducing sugars) can really introduce a difference in the thermodynamic behaviour of the downstream processes. Thus, the objective of this work is to present a downstream process configuration design for acetone, butanol and ethanol separation. The methodology followed started with the thermodynamic data collection and the operating conditions for the separation process.[1] The mixture concentration entering to the separation section contains all the compound leaving the fermentation section such as water, acetone, butanol, ethanol, carbon dioxide, glucose, etc. This data was obtained from some results at lab scale[4] and some literature on the modelling fields. The downstream section consist of four distillation columns, the first is employed to separate most of the water and glucose at the bottom of the column; on the second column, the butanol is obtained at the bottom with a purity of 98.8 wt %. The following distillation column was employed to separate most of the ethanol and remaining water; and the last column was employed to obtain the acetone at the bottom with a purity of 93.4 wt%. The calculations were performed using the computer-aided simulation tool PRO/II v 9.0 (Invensys Systems Inc.).

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[666]

Financial Considerations in Shale Gas Supply Chain Development

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In this work, an optimization framework to support the planning of the development of shale gas resources is proposed. Financial aspects are taken into account through the integration of financing options, such as own capital, and external sources, short and long term bank credit lines. The model also includes the design of well-pads in terms of total number of wells, and length and number of hydraulic fractures completed at each well. In addition, different capacities and locations are considered for compressor stations, gas separation plants, and water treatment plants. A case study involving two alternative financing strategies was conducted to demonstrate the capabilities of the model. It is found that external financing can play an important role in the development of a shale gas field, achieving an increase in net profit of almost 65 % when compared to a scenario where only own capital is considered.

[668]

Optimal dynamic operation of adsorption-based energy systems driven by fluctuating renewable energy

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Adsorption-based energy systems have the potential to provide environmentally friendly heating and cooling energy as they can be driven by low-grade heat, such as solar or waste heat. However, solar and often also waste heat are fluctuating over time. Thus, an optimal operation policy has to be found to run the adsorption-based energy system efficiently. Thereby, the intrinsic dynamics of the adsorption-based energy systems have to be considered: These processes are usually cyclic switching between adsorption and desorption phases.

This work therefore presents a method to determine the optimal operation control for dynamic adsorption-based energy systems. To determine the optimal control, a two-step approach is used: First, the original dynamic model, consisting of ordinary differential and algebraic equations (DAE-model) is approximated by a set of linear ordinary differential equations (ODEs) connected by Heaviside functions. In a second step, the approximated model is optimized for a set of control variables using a gradient method.

In the present work, a DAE-model for a solar cooling adsorption chiller is used. We analyze the sources of uncertainty of our method by studying the influence of the linearization point, the Heaviside function and the boundary conditions. The method is shown to reliably provide the optimal control and to be robust for a wide range of the investigated parameters. Finally, the optimal operation of the chiller is determined for an example day.

[671]

A Spatial Multi-Period Mixed Integer Linear Programming (MILP) Model for Optimal Power Planning: CO2 Emissions Mitigation

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According to the Exxon Mobile Energy Outlook (Exxon Mobile, 2014), worldwide electricity use is expected to grow by 90% from 2010 to 2040. Developing countries account for about 85% of that increase. Therefore, power planning is an important issue in order to provide reliable and sustainable secondary energy in timely fashion, particularly in developing countries. Consequently, energy and power planning problems have capture the attention of the academic research community (Sirikitputtisak et al. (2009), Mirzaesmaeeli & Elkamel (2010), Koltsaklis et al. (2014), and Flores et al. (2014)).

In this work we present a spatial multi-period MILP optimization model for optimal power generation expansion planning. The model includes spinning and non-spinning reserve constraints, as well as CO2 emission constraints. Carbon Capture and Sequestration (CCS) technologies are considered for both existing and new fossil power plants, in order to meet CO2 emission reduction targets. The model also accounts for transmission capacity and cost for power transfer between the interconnected regions. In addition, lead time is considered for construction of new power plants, since such lead times can be quite long. The novelty of the proposed model relies on an integrated assessment of the aforementioned features, which can reveal possible interactions and synergies within the power system.

The main capabilities of the proposed model are demonstrated through a real world case study related to the Colombian electric power system, which has a total of 40 existing power plants distributed between 5 interconnected regions. Existing power plants include 22 hydroelectric, 15 natural gas and 3 coal power plants. Total installed capacity is about 13,717 MW. Electricity demand for that system is expected to increase about 50% in the next 15 years. Consequently, new power plants, including coal and natural gas plants, need to be integrated into the system, potentially significantly increasing the total CO2 emissions. The reduction of CO2 emissions can be addressed by the implementation of CCS technologies in existing and/or future power plants. Here, different CO2 emission reduction scenarios are considered and economic implications in terms of incremental increase in electricity production cost ($/MWh) are identified.

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[683]

Bringing non-energy systems into bioenergy value chain optimization framework

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Energy sectors are responsible for over 80% of the total greenhouse gas (GHG) emissions in the EU-28 [1] and approximately 83% of the UK GHGs in 2012 [2]. Bioenergy has been widely recognized as a strategy for mitigating climate change. This has triggered ambitious national/regional policy targets mandating the bioenergy roles within the overall energy portfolio e.g. the RED target of a 20% share of renewable energy in the EU energy mix by 2020 [3]. However, bioenergy is a complex system, which involves many interrelated or conflicting issues e.g. economic development vs. environmental and social sustainability, interaction of energy with food sectors. Thus the large scale deployment of bioenergy requires a thorough understanding of how whole bioenergy value chains perform and the interaction of multiple systems relying on the same resources.

This study presents a multi-objective optimization model configured to account for a range of interrelated or conflicting issues involved in bioenergy systems. A spatial-temporal mixed integer linear programming model - ETI-BVCM (Energy Technologies Institute - Bioenergy Value Chain Model) [4] - was adopted and extended to incorporate resource-competing systems (bioenergy vs. non-energy) and effects on ecosystem services (ES) brought about by the land use transition in response to bioenergy penetration over five decades. The extended model functionality allows for exploring the effects of constraining ES impacts on other system-wide performance measures such as cost or GHG emissions. The users can therefore constrain a metric which quantifies (to a certain extent) the change in ES from land use transitions. The developed model provides a decision-making tool for optimal design of bioenergy value chains supporting an economically and land-use efficient and environmentally sustainable UK energy system meanwhile delivering multiple ES. The study demonstrates the types of valuable insights the extended optimization modelling framework could provide for policy formulation to accelerate bioenergy penetration and support its sustainable development.

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Biorefinery Process Optimization and Risk Estimation at Industrial Level

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Biofuels constitute an attractive alternative to complement fossil fuels. In this context, significant growth has been generated in different countries for biodiesel production, to meet both internal and external demand for home consumption. Biodiesel production using microalgae as feedstock has shown several advantages; however, it comprises a series of processes that must be properly evaluated. Technology development and process optimization are necessary to minimize the overall production cost. Moreover, in the framework of process sustainability, social and environmental impacts should include risks assessment by means of the consequences estimation. Therefore, it is mandatory to be familiar with the characteristics and hazards of the chemicals and processes, as they may cause unsafe operating conditions and lead to accidents dangerous for human health and the ecosystem.

The purpose of this work is the development of biodiesel production processes with microalgae as feedstock and the subsequent technological risk assessment, thus contributing to more sustainable and safe processes. In order to reduce external energy and nutrient requirements, the biorefinery process is optimized, assessing several additional steps to the biodiesel production process with microalgae: anaerobic digestion, CO2 depuration and generation of thermal and electrical energy [1]. In this sense, the input parameters are evaluated and selected to develop a proper model, looking for the optimization of the following processes: algae cultivation, flocculation and separation, oil extraction, transesterification, anaerobic digestion, purification of CO2 and generation of thermal and electric energy. On the other hand, a quantitative risk assessment is performed to move forward on industrial risks associated to the biodiesel production using as feedstock microalgae and a low molecular weight alcohol. Hazardous substances were identified in the process, simulating the consequences of different leaking scenarios. The major risks detected were: fire involving biodiesel and fire, explosion and toxic dispersion of methanol [2]. The obtained results are evaluated and will support the future decision-making, determining optimal operating conditions and estimating the consequences and the associated cost.

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[704]

MILP approach for the design of residential microgrids with energy interaction restrictions

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Distributed generation units (DG) and microgrids (MG) have the potential to enhance the use of locally available renewable energy resources in residential areas, addressing both the growing global energy needs as well as emission reduction targets. For MGs and DGs to appear on a large scale, however, the design and operation of residential distributed energy systems (RDES) should be cost effective, reliable and efficient. RDES are often able to export electricity to the central distribution grid to prevent overloading through excess local generation or to create an income through governmental support schemes. Electricity export restrictions thus bound the potential income and behaviour of RDES. Proposed regulatory changes to cut residential electricity export allowance coupled with efforts that are needed to upgrade existent distribution grid infrastructure to allow for un-restricted bi-directional electricity flows are expected to challenge the design and operational characteristics of RDES.

This study presents a deterministic superstructure approach for the techno-economic optimisation of such optimal neighbourhood design in terms of location, sizing and operation under various levels of electricity export allowance. A mixed integer linear programming approach is adopted that minimises the total annualised cost for the neighbourhood as a whole to meet its yearly energy demands including space cooling, space heating and electricity. The total energy demand in the neighbourhood is satisfied by the consideration and combined use of conventional and DG technologies such as condensing boilers, gas heaters, air-conditioning units, photovoltaics, small scale wind turbines, combined heat and power units and absorption chillers together with energy storage units and an optional interconnection with the centralised grid. Each unit is modelled as a black box characterised by its performance parameters. Moreover, a pipeline network can be installed to allow for heating and cooling integration of the neighbourhood in multiple non-circulating networks. Additionally, electrical integration of the site can be achieved through the installation of a MG without internal feedback loops. A case study framed by South Australian climatological, economic and regulatory characteristics is presented employing an hour based interval of typical days over a yearly planning horizon. The purpose of this study is to analyse the impact of electricity export restrictions of the RDES to the central electricity grid. Additionally, energy circulation restrictions between households are analysed through energy system design constraints. This is motivated by a proposed change in Australian energy regulations to cut residential electricity export.

The proposed methodology incorporates an energy integrated superstructure approach of RDES which focusses not only on electrical integration or heating integration of the neighbourhood but encompassing a full integration of electricity, heating and cooling without internal feedback loops. Both electricity, hot and cold storage as well as different technologies to meet each of the energy demands are accounted for. The presented approach identified optimum characteristics leading to cost effective and sustainable residential energy system design under various electricity export levels. The importance of electricity export and advisable levels are highlighted through the study of selected energy system design scenarios of the residential site.

[723]

Engineering Design of Localised Synergistic Production Systems

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With the advent of industrialisation, the supply of energy and materials to meet human needs has shifted from distributed production based on locally available resources to centralised production based on fossil fuels and large scale distribution infrastructures. However, continuation of this mode of production, coupled with rising economies and growing population and the subsequent increase in the demands for essential commodities and services, has led to a plethora of issues such as energy supply insecurity, climate change; deterioration of ecosystems, social-economic injustice and depletion of resources. The motivation of this research is that the establishment of localised production systems can potentially reduce unsustainable resource consumption and negative environmental impact for meeting local needs and bring other socio-economic benefits. If designed in a systematic way, they can represent a possible pathway towards sustainability. Therefore, the main objective of this work is to develop engineering tools for the design of efficient local production systems.

A local production system is defined in this work as a network of heterogeneous processes, including both technological and ecological, integrated in a synergistic manner to achieve a high degree of resource efficiency, potentially leading to improved economic viability while preserving the ecosystem. The geographical boundary of a local production system can be considered as that of an area under the direct governance of a local or regional planning body. The main components of the local production system are ecosystem, production (including resource extraction) and consumption. Such a production system has the potential to facilitate more effective use of local renewable energy sources and to allow rational alignment of resource, production and consumption within the same locality, avoiding the burden of large transportation distances and enabling close integration between different processes and flows.

We propose to design a local production system with the objective of minimising total resource consumption given a set of local demands to be met by a proper combination of available resources and processes while observing a set of ecological and technical constraints. In order to find a solution to such a design problem, a simultaneous or an incremental design approach could be applied. In this work, we focus on an incremental design approach by which multiple production system components supplying different products or services are introduced sequentially with necessary iterations; the design sequence is determined according to the relative independence of each system component. The total resource consumption is expressed as cumulative exergy consumption which can be calculated using the Cumulative Exergy Resource Accounting methodology. This methodology takes into account cumulative consumption of capital and operating resources as well as resources needed for environmental remediation (i.e. for treating harmful effluents). The design approach will be illustrated through the co-design of energy, water and food production with reference to the locale of an eco-town in the UK.

[729]

Modelling multi stream heat exchangers using operational data

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Multi stream heat exchangers (MSHE) are single process units that facilitate simultaneous exchange of heat among multiple streams. They are widely used in cryogenic processes such as air separation and LNG. MSHEs are generally complex, proprietary, and involve phase changes of mixtures. Existing MSHE models in the literature involve disjunctions and result in complex MINLP models that are computationally expensive. Since they must be solved repeatedly inside an optimization framework of the entire process, there is a need for simpler models that can effectively capture the phase change phenomena. In this work, we present a simpler superstructure of 2-stream exchangers to describe an MSHE and propose a simpler formulation without any disjunctions to obtain a best fit for given operational data.

MSHEs use several bundles in a series and streams may transition through all operational regimes, viz. super-heated, two-phase and sub-cooled. The Temperature-Enthalpy (T-H) curve is significantly different for each phase and heat exchanger coefficients vary substantially for each operating regime. To handle phase changes, Hasan et al [1] proposed the idea of using a hypothetical network of 2-stream heat exchangers to represent MSHE operation, and developed a novel mixed-integer nonlinear programming (MINLP) formulation. However, they allowed multiple exchanges between a hot stream and the cold stream, resulting in a complex network. Also, they assumed no pressure drop in a bundle and did not account for components like J-T valves. Alternatively, Kamath et al. [2] presented an equation-oriented model that relies on the pinch concept to ensure minimum driving force and regarded MSHE as a special case of a network with no utilities. They proposed a disjunctive formulation to detect phases and perform appropriate flash and enthalpy calculations. To account for the pressure drop, they made a simplifying assumption that the pressure varies linearly with the heat load of the stream.

In this work, we propose a novel superstructure of 2-stream heat exchangers based on the operational regimes of the exchanging streams. We use operational data to identify these operational regimes in each bundle, and place 2-stream heat exchanger/s between portions of hot streams and the cold stream. Also, we avoid multiple heat exchanges between a hot stream and the cold stream to ensure simplicity, and allow components like J-T valves in the HE-network to represent the reality better. In addition, we accurately account for the pressure drops in the MSHE bundles. Our approach enables us to fully deduce a suitable network without the need for any disjunctions, making our formulation NLP rather than MINLP. This significantly reduces the complexity of the problem and makes this work very useful for the optimization of the entire process. Finally, we demonstrate the usefulness of our approach on a MSHE from an LNG plant and compare our network with those from the literature.

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[777]

Improving the Energy Efficiency of Cryogenic Air Separation Units (ASU) through Compressor Waste Heat Recovery using Direct Binary Heat Engine Cycle

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Cryogenic Air Separation Units (ASU) forms an integral part of many industrial processes due to its ability to generate high tonnage and high purity useful gases (nitrogen, oxygen and argon) to many industrial processes. Oxygen is widely used in medical, metal processing, ammonia, power generation, glass industries etc., nitrogen finds use in chemical and petroleum industries while argon are mainly used for inert shielding gas in welding and light bulb. However, the process is an energy intensive process.

In a typical cryogenic ASU, about 90% of the energy in the form of electrical energy is consumed by the air compressor. The compression of the air provides high temperature compressed air at the compressor effluent. These high temperature air are useful heat resources which can be recovered for electricity generation using a direct binary heat engine cycles otherwise known as Organic Rankine Cycles (ORC).

Thermodynamic analysis carried out through modeling and simulation using Aspen Plus® shows that the recovery of compressor waste heat from a cryogenic ASU using ORC system reduces the overall electricity consumption of a conventional ASU by 11%. This translates to a displacement of about 2.15 x 10^7 kgCO2/year from the environment had it been the electricity were generated using a conventional coal fired power plant.

[834]

IGCC Modelling for Simultaneous Power Generation and CO2 Capture

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Power producing industry has largely relied on coal as a fuel source and will continue to depend on it for coming decades. However, addressing the global warming problem while keeping high efficiency and economic feasibility of the processes is a key challenge. Coal-based power plants with post-combustion capture tends to have lower capital costs and cost of electricity without capture. On the other hand, pre-combustion capture plants tend to be less expensive when current CO2 capture systems are added. This analysis suggests that pre-combustion plants can be an attractive option for the power generation if CCS technology is implemented on a large scale. This paper is focused on the in depth modeling and simulation of integrated gasification combined cycle (IGCC) with CO2 capture using a physical solvent. Three case studies have been developed to analyze the overall plant output with CO2 capture. In order to ensure a fair evaluation of analysis, a consistent and transparent methodology has been followed for all the cases. First two cases use the water gas shift reactions scheme with sour shift catalysis process as described. The resulted syngas free of CO2 can either be combusted by using air or O2. The case 1 uses air as an oxidant for burning H2 and the combustor temperature is controlled by air as well. For case 2, O2 is used as an oxidizing agent in the H2 combustion. However, combustion temperature control is achieved by using CO2. In the case 3, water gas shift (WGS) reactor has been removed The syngas composed of CO and H2 is sent directly for combustion which makes it similar to the oxy-fuel combustion process. Case 3 uses CO2 to control the combustion temperature. In this way, captured CO2 can be recycled back to control the combustor temperature in case 2 and 3. The results show that the overall plant output power for case 1, 2 and 3 is 478 MW, 416 MW and 460 MW respectively. Case 1 and case 3 are the competitive options in terms of efficiency; however the capital cost may be the deciding parameter.

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[841]

Preliminary analysis of systems for integrating solar thermal energy into processes with heat demands

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The solar energy is one of the more widely available renewable energy sources. The solar source is received by the Earth for free, however harvesting the thermal energy requires appropriate hardware and related investment. This lead to the development of numerous solar collectors with different characteristics and prices. A preliminary selection with preliminary assessment of the system should be performed before making detailed analyses for all the available integration when planning an energy system. Only those solar thermal integration systems that promising an appropriate trade-off between the integrated amount of energy from solar source and investment should be considered for further planning.

The aim of the current work is to develop a method for preliminary evaluation of the trade-off between the integrated amount of solar thermal energy, into processes with heat demands, and the investment. A targeting method has been developed for maximising the amount of integration of thermal energy processed by the optimised size of solar collector surface area as well as the size of heat storage has been developed. The size of the solar collector area and heat storage is based on the number of consecutive sunny days and not sunny day. In the first step the data of the heat demand are collected. Heat demands which can be potentially satisfied from the solar source are specified. In the second step the amount of heat per surface area unit was determined as gained during sunny day (area-specific heat). The collector system and geographical characteristics are taken into account when determining the amount of heat gained. The temperature driving forces are taken into account for heat exchanges between solar collector medium and storage and also between storage and process demand. The required collector surface area is defined as the heat demand for the sunny and not sunny days together divided by the product of area-specific heat of a given collector an the number of sunny days at a given geographical location.

The proposed targeting method can be applied for the pre-screening of alternatives in order to eliminate economically not viable solution before more detailed system synthesis is performed.

[849]

Structural Similarities and Differences between Smart Grids and Process Industry Supply Chains: India Case Study

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Process industry supply chains have been an active area of research for decades with advances towards decentralized management and development of closed loop resilience. Along similar lines, now electric power systems are moving towards smart grids that allow for decentralized power generation. At the surface level there are many differences between electrical grids and supply chains; for example, there is limited/no storage in case of electric power, hence supply and demand has to be matched at every time instant. Recently it has been recognized that the some of the control and enterprise-wide optimization strategies that are an integral part of supply chain management have analogues in power systems as well. This paper seeks to systematically identify the structural similarities and differences between these hitherto unrelated domains. We will illustrate these using a case study of Indian electrical grid.

The traditional approach to system management in both the supply chain and electric power domains have been (1) uni-directional flows (of material and electric power), (2) near steady supply and demand with low volatilities, (3) use of large inventories (material / spin reserves) at various stages of the system to balance supply and demand, and (4) low uncertainties. More recently, driven by sustainability-related and other considerations, both systems are undergoing an evolution towards (1) bi-directional flows (for eg: closed loop supply chains and distributed generation capabilities), (2) uncertain and highly variable supply and demand.

The broad strategies that the two domains have evolved to address these challenges and ensure effective system management also share broad similarities and originate from recent developments in ICT and sensing. These similarities are (1) frequent, two-way information exchange between supplier and production, production and distribution, and distribution and customers; (2) shifting from centralized decision making to decentralized decision making; and (3) exploiting spatial and temporal flexibilities.

In this paper, we will systematically map the similarities and differences between these different domains. Based on this analysis, we will project the learning around optimization and decision making that has originated in the supply chain domain to the electrical power systems. We will also offer a perspective on unique challenges that afflict the power network (eg: small time constants, limited inventories, etc) and modifications necessary to the existing supply networks related technology for them to be applicable in the arena of power networks. Finally, we will illustrate all the features, similarities, dissimilarities, extendibility of solutions and challenges using the case study of the Indian electrical grid.

[850]

Integrated Computational and Experimental Studies of Microalgal Production of Fuels and Chemicals

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In recent decades, it has become obvious the reliance on traditional fossil fuel resources is unsustainable, due to both the irreversible depletion of fossil fuels and the associated greenhouse gas emissions which cause global warming (Hoel and Kverndokk, 1996). Microalgae are sunlight-driven cell factories that carry out the same process and mechanism of photosynthesis as higher plants converting sunlight into biomass, but they perform more efficiently than crops (Chisti, 2007). Nevertheless, high substrate and fertilizer input requirements as well as harvesting and oil extraction cost have been found to play a significant role in both the economic viability and sustainability of microalgal biofuels production (Pittman et al., 2011). Therefore, attention has been drawn to experimental and computational studies on the microalgal oil production in the scientific milieu which aims to increase the productivity either through the photosynthesis process or through the application of metabolic engineering to microalgae (Chisti, 2007) and also to improve the sustainability and competitiveness of the algal-derived biofuels industry. The objective of this work is the establishment of links between algal strains grown in large raceway open ponds and innovative bioproduct generation technologies including fuels and chemicals in order to achieve positive energy balance and environmental sustainability. A multi-parameter quantification leading to a predictive model has been employed to describe algal growth and lipid accumulation in lab-scale batch systems. The model can also take into account the effects of temperature, light and pH (Zhang et al., 1999) in order to improve the productivity of microalgae cultivation technologies. Experiments have been conducted to analyse the effect of different input parameters. Furthermore, an in-house developed global optimization framework (Vlysidis et al., 2011) is employed for the estimation of key parameters used in bench-scale batch systems.

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Process Integration and Assessment of Biogas System

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Anaerobic digestion and biogas production are promising means of producing an energy carrier from renewable resources [1]. Biogas is arguably a more versatile renewable energy source due to its determinate energy value and ease of storage, hence, potential utilization is significantly independent of factors such as geographical location and season. It can be used directly for heating and electricity generation, and as substitute for fossil fuel applications, e.g., natural gas, transport fuel [2]. However, from a system analysis perspective, biogas production is a complex system which covers different activities, such as the collection and pretreatment variety of available raw materials, digestion technologies, biogas upgrading, digestate treatment and biogas utilization. Thus, integration of the whole system considering its energetic and environmental performance is important for the technology development and industrialization of the biogas.

In this work, we established the material and energy flow charts of a base senario which contain several units including biomass collection & transportation, pretreatment, anaerobic fermentation, biogas upgrading and digestate treatment and utilization. According to the system energy balance, we calculated the LHV based system energy efficiency which contains the biomass feedstocks' LHV [3]. We chose the anaerobic digestion and biogas upgrading units as the key units and investigated various technologies' combination and some energy and steam recycling to the effect of the biogas system's energy and material efficiency. Finally, the Green Degree (GD) [4] based environment evaluation was conducted which considering the Global Warming Potential, Ozone Depleting Potential, Acidification Potential etc., giving a comprehensive assessment of the biogas system from both the energetic and environmental aspects.

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[887]

Development and Parameter Estimation for a Multivariate Herschel-Bulkley Rheological Model of a Nanoparticle-Based Smart Drilling Fluid

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Smart drilling fluids containing FeO nanoparticles have advantages toward increasing the energy and hydraulic efficiency of drilling operations in reservoir environments. Exploring and optimizing the rheological behavior of such new drilling fluids is critical, implying direct and significant economic savings in developing new oil and gas fields. A experimental campaign analyzing the rheology of a bentonite-based fluid produced a new multiparametric dataset, considering a wide range of realistic reservoir conditions. Non-Newtonian behaviour is confirmed by yield stress computation for all these cases. Heating and rotation induce temperature and concentration gradients at drilling depth: it is hence essential to obtain an accurate but also versatile multivariate rheological model, which will enable viscosity prediction for the analyzed and other similar drilling fluids. The enhanced Herschel-Bulkley model is developed on a multiplicative assumption, postulating and analysing candidate equations which quantify the effect of shear rate, temperature and nanoparticle concentration on drilling fluid shear stress and viscosity. Parameter estimates have been subsequently determined via systematic optimisation, using statistical metrics to quantify and compare uncertainty and predictive potential. The trivariate shear stress and viscosity models proposed are similar in form: each requires six parameters used to combine a Herschel-Bulkley yield stress expression, an Arrhenius exponential of temperature and a linear model for nanoparticle concentration.

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[893]

Design of Rankine cycles for waste heat to power conversions in Carbon Capture compression trains

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Multi-stage compression systems are power intensive and produce significant amounts of low to medium grade waste heat that is typically rejected into cold utility during the intercooling steps. The recovery and reuse of this waste heat is a potential option to enhance overall process energy efficiency. Organic Rankine Cycles (ORCs) allow to convert such low to medium grade heat to power at improved efficiencies as compared to steam cycles. This work focuses on the design of ORCs to recover waste heat for power generation from intercooling operations so as to offset the overall power intensity of multi-stage compression trains.

The application focus of the work is waste heat recovery and conversion to power in carbon capture compression trains. Compression trains are an essential part of carbon capture process plant, where the carbon dioxide is compressed to the pressure of saturate vapour after it has been liquefied. The compression train is a significant contributor to the overall cost of the carbon capture system as it requires a substantial amount of power. The heat removed in the intercoolers is of low grade heat with temperatures below 180°C, which renders ORCs a promising option for its conversion to power. The generated power is used to partially offset the overall power requirements of run compression train.

We present and apply a method to design ORC configurations for power geenration from the various streams in between compression stages, which implements the exergy composite curves approach to explore the problem as part of an optimization formulation. The method allows generating and evaluating different ORC configurations on the basis of a newly proposed objective function based solely on thermodynamic criteria to determine the preferred options. Results will be presented and design insights derived from the application of the presented approach to design ORC configurations for a typical carbon capture compression train.

[917]

Adaptive Management of Renewable Energy Smart Grids Using a Power Grand Composite Curves Approach

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Hybrid energy smart grids operate based on power management strategies (PMS) addressing the time-varying reallocation of resources to meet specific targets. The identification of the PMS that best exploits the weather variability is crucial for their efficient operation. In this work, this is approached within a framework which exploits the Power Grand Composite Curves (PGCC) method to perform two functions: a) the identification of renewable energy recovery targets within a short term prediction horizon, and b) the temporal reallocation of the grid subsystems within a control horizon based on the PMS that best matches the identified targets. The PGCC is exploited within a model predictive control framework that enables the satisfaction of the system operating goals by ensuring the maintenance of a targeted minimum energy inventory. The desired energy inventory is guaranteed by selecting the appropriate PMS during the control interval that best matches the identified target. The method is presented within a formal mathematical framework and illustrated for a smart grid with power and hydrogen generation and storage features in year-round operation.

[930]

Impact of the operating conditions and position of exhaust gas recirculation on the performance of a micro gas turbine

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Gas turbines are a viable and secure option both economically and environmentally for power and heat generation. The process simulation of the micro gas turbine with exhaust gas recirculation (EGR) and its impact on performance is evaluated. This study is further extended to evaluate the effect of the operating conditions and position of the EGR on the performance of the micro gas turbine. The performance analysis for different configurations of the EGR cycle, as well as flue gas condensation temperature, results in the optimized position of EGR at the compressor inlet with partial condensation resulting in the CO2 enhancement to 3.7 mol%.

[957]

Dynamic Response of Fuel Cell Gas Turbine Hybrid to Fuel Composition Changes using Hardware-based Simulations

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The solid oxide fuel cell gas turbine hybrid system (SOFC/GT) is an exciting new approach to producing electricity with high efficiency and lower environmental impacts than conventional power plants. One of its key strengths is the potential for fuel flexibility, which is the ability to transition between different kinds or qualities of fuels during operation. However, there has been very little research into the dynamic performance of SOFC/GT systems in response to changes in fuel. Therefore, the open loop behaviour of SOFC/GT systems in response to fuel composition transients was experimentally investigated. In this study, hardware-based simulations were used to study transitions between using coal-derived syngas and humidified methane. A hybrid test facility at the U.S Department of Energy, National Energy Technology Laboratory, Morgantown, West Virginia, was used to adequately capture the coupling of fuel cell stacks (simulated with a real time dynamic model) and a gas turbine system (from actual equipment) during transient events. Given the dynamic trajectories of key process variables, the impact on the hybrid system was quantified via transfer functions. The results show that the open-loop dynamic behaviour exhibited significant inverse response which limited the range of transitions that could be achieved safely without damage to various system components such as the compressor or fuel cells. However, the results also showed that if a control system could be designed which limited the impact of the inverse response, then transitions between even very different kinds of fuels could potentially be achieved without operational problems. The resulting transient information will be used to develop a new control system for thermal management of SOFC/GT hybrid systems in future work.

[966]

Short-term planning of cogeneration power plants: a comparison between MINLP and piecewise-linear MILP formulations

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A Combined Heat and Power (CHP) plant, or cogeneration power plant, is an energy system composed of a network of units that convert primary energy into electricity and heat. The system may include not only cogeneration units, that generate simultaneously heat and electricity, but also other generation units and heat storage tanks.

The optimization of cogeneration systems has great practical relevance and gives rise to a wide range of problems that have received a growing attention during the last decade. Among them, the short-term operation planning problem consists in determining, for each period t of a finite time horizon, which units must be switched on/off, the value of their operating variables (e.g., input fuel), and the amount of stored energy, in order to minimize an objective function (e.g., the total operating costs), while satisfying the demands of electric, thermal and refrigeration power. The performance curves of the (co)generation units are, in general, nonlinear. A number of additional constraints may also exist, such as upper bounds on the number of start-ups. As a result, the problem turns out to be a challenging mixed-integer nonlinear program (MINLP).

In this work, we compare two solution strategies: the first strategy consists in formulating and directly tackling the MINLP, while the second one is the approach proposed by (Author, 2014) based on state-of-the-art linearization techniques (piecewise-linear approximation of the nonlinear performance curves, big-M constraints, etc.) so as to obtain a mixed-integer linear program (MILP). Both models are implemented in AMPL, and the MINLP is tackled with BARON, whereas the MILP is solved with CPLEX.

The two strategies are tested on a set of real-world problems representative of both residential and industrial applications.

Computational results are analyzed with reference to computational time and solution quality. The MINLP formulation is already challenging for instances with a few units, and guaranteeing optimality seems out of reach for all but the simplest instances. The piecewise-linear approximation allows solving larger-sized instances to optimality in significantly less time, even when the approximation is fairly accurate.

[978]

Optimum Facility Location and Plant Scheduling for Biofuel Production

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Biomass is an abundant, locally available, and renewable raw material for liquid fuel production. The biomass-to-biofuel supply chain (BTBSP) contains biomass growth, biorefineries, and demand centers. The optimum design and operation of this supply chain is crucial for cost effective production of biofuels, and there are ample studies in the literature that focuses on optimizing the location and size of biorefineries for selected geographical regions. For example, Marvin et al. [1] presented a MILP for ethanol production in a 9-state region in the Midwest. Giarola et al. [2] presented a similar model for Northern Italy, and examined a multi-objective problem also minimizing GHG emissions. However, most models assume a certain amount of biomass availability, and hence, fail to consider the overall BTBSC. Cost of biomass growth accounts for a significant portion of the biofuel production cost, and the optimal design of BTBSC should also include the batch-like characteristics of biomass growth.

In this paper, we present a mixed integer linear program (MILP) for optimal design of BTBSC with biorefinery location and capacities, and campaign plan for biomass production. The objective of the model is to maximize the net present value (NPV) of the overall supply chain over the planning horizon. The NPV includes biomass growth costs, capital and operation costs for biorefineries, and transportation cost between the locations of biomass growth and biorefineries, and between biorefineries and demand centers. The addition of biomass-growth campaign planning allows the possibility of incorporating seasonality, crop-rotation, and feedstock diversification at the BTBSC design stage. The model includes multiple potential feedstock crops, and production pathways to both cellulosic ethanol and biodiesel, and determines the optimal biorefinery locations and corresponding capacities, and the biomass-growth campaign plan.

The case study consider the design of BTBSC for a region encompassing 18 counties of the State of Oklahoma for 10 years. Switchgrass, indiangrass, big blue stem, poplar, soybean, sunflower seed and rapeseed are selected as potential biomass resources. Cellulosic ethanol can be produced by two process platforms: enzymatic hydrolysis or acid hydrolysis followed by fermentation and gasification. For producing biodiesel, only supercritical transesterification technology is considered. Biomass is assumed to be transported by 22.7 wet metric ton load semi-trucks. Bioethanol and biodiesel are assumed to be transported via rail transportation. Biofuel demands are forecasted using 4-year moving average of historical population and gasoline and diesel consumption data. The MILP is modeled in GAMS, and has 581,845 constrains and 961,015 variables. The solution recommends planting in Tulsa region, with biorefineries that produce bioethanol in all 18 counties. 68.4% of biomass is converted to produce 9.42E+8 gal of bioethanol for 10 years.

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[991]

Energy consumption scheduling of smart homes with microgrid under multi-objective optimisation

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The global electricity increases by 2.4% annually and the price of fossil fuels has increased quickly during the last decade. More countries are concerned with reducing energy cost and emissions. Microgrid is regarded as an alternative to the current centralised energy generation systems. It can provide economic benefits through avoiding long-distance transmission. Environmental benefits can be obtained by utilising distributed energy resources (DER) with low pollutant generation. Meanwhile, security and reliability can be gained from interconnection and coordinated control. Smart homes are becoming popular for their lower energy cost and provision of comfort and the rapid advances in computing and communication capabilities promote the concept. Flexible energy-consuming household tasks can be scheduled co-ordinately among multiple homes which share the common microgrid. The economic cost and CO2 can be both reduced. However, the electricity tariff is not always positively correlated with CO2 intensity and they may conflict with each other.

In this work, a mixed integer linear programming (MILP) model is proposed to schedule the energy consumption within smart homes. The daily power consumption tasks are scheduled by coupling environmental and economic sustainability in a multi-objective optimisation with ε-constraint method. The two conflict objectives are to minimise the daily energy cost and CO2 emissions. DER operation and electricity-consumption household tasks are scheduled. The proposed model is implemented on a smart building of 30 homes. Electricity tariff and CO2 intensity profiles of Ireland and UK are employed for the case study. The Pareto curves for cost and CO2 emissions present the trade-off between the two conflict objectives. The results indicate the possibility of cost savings and emission reduction through the daily power consumption tasks scheduling and better management of DER operation.

[1007]

Optimization of pressure/vacuum swing adsorption with variable dehydration levels for post combustion carbon capture

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In 2010, 30.6 gigatons of CO2 were emitted into the atmosphere worldwide, with around 38% of the emissions in the US coming from the generation of electricity [1]. To reduce these emissions, there are substantial efforts to develop renewable energy technologies with minimal net carbon emissions. However, over the next few decades, fossil fuels will continue to play an important role in our energy mix [2]. Therefore, there is significant interest in reducing the CO2 emissions from existing power plants via Carbon Capture and Sequestration (CCS). Of all the technologies available for CCS, Pressure/Vacuum Swing Adsorption (PSA/VSA) is perhaps the most promising due to its higher performance and lower energy requirements compared to the other technologies [3]. This has led to increased interest in PSA/VSA cycles for carbon capture. However, in the majority of recent publications, the inlet flue gas stream is assumed to contain no water. In reality, flue gas from power plants is usually saturated with water, containing around 3-5 mol%. Recently, it has been shown that certain metal-organic frameworks (MOFs) are stable under humid conditions but with diminishing CO2 loading as the humidity level increases, allowing the possibility of partial dehydration of the stream[4]. The goal of this work is to determine the optimal dehydration level for various MOFs and zeolites, with the minimum cost, including dehydration costs, while maintaining the desired process performance.

In this work, various PSA/VSA cycles including a two-stage Skarstrom cycle, are analyzed using mass and energy balance equations along with adsorption isotherms of selected MOFs. The tradeoff between dehydration cost and performance is examined by allowing the concentration of water to vary. This is coupled with material selection from several promising adsorbent candidates including HKUST-1, CPO-27, zeolite 5A, and zeolite 13X. Through the inclusion of the impact of water on CO2 uptake for each material, the optimal material and water level are determined. Finally, the overall cost of the process is calculated in order to compare the performance of the different materials. These costs include dehydration costs, estimated costs of the adsorbent and operating costs. Since the goal of lowest costs along with the constraints of the desired process parameters are competing goals, a multi-objective non-dominate sorting genetic algorithm II (NSGA-II) is used to develop a Pareto front of the annualized cost of the system and the purity of the CO2 product. The objective of the work is to minimize the overall cost of capturing CO2 from the flue gas along while maintaining a high purity of the final product.

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[1091]

Process Synthesis for the Recycle of Spent Lithium Ion Batteries by Chemical Precipitation

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The recent increased use of lithium ion batteries (LIB) inelectronic equipment and electric vehicles has significantly increased thenumber of spent batteries. It is crucial that the various components in LIB berecovered and reused. Cathode materials that contain Li and other metals arethe obvious targets for recycling. In such a process, metal ions are firstdissolved from the cathode plate, followed by separating and recovering metalsalts from the solution in various steps. Acids such as dilute HCl, HNO3,and H2SO4 could be used to dissolve metal ions from thecathode plate. The dissolved metal ions are then separated and recovered byvarious processes such as electrochemical process, chemical precipitation, andsolvent extraction. Among these recovery techniques, chemical precipitation iscommonly employed. The metal salt recovered from the precipitation process canbe a mixed metal oxide such as LiCoO2 or a compound containing a singlemetal salt such as Li2CO3. However, it is not easy to controlthe target products to be recovered from the precipitation process. The majorreason is that the operating conditions for these precipitation processes aredetermined by trial and error, without considering the solid-liquid equilibrium(SLE) phase behavior that governs the chemical precipitation process. Withoutunderstanding the phase behavior of these systems, compounds other than thetarget compound(s) may be recovered from the precipitation process. Or, the targetcompound would co-precipitate with other metal salts, leading to a reduced purityof the compound recovered from the process or a more complicated process to furtherseparate the mixed metal compounds. Even if the target compound is precipitated,the operating conditions may not be the optimal, leading to a lower recovery inthe precipitation process or excess usage of chemicals. The process developedbased on trial and error is also very specific, meaning that the process may notbe applicable even if the same cathode material, but with a differentcomposition, is recycled. One example would be the ratio of Co and Mn ischanged from 1:9 to 9:1 in LiCoxMn1-x cathode material. The utilization of SLE phase behavior to design precipitationprocesses is well developed in the literature. Wibowo and Ng developed aunified procedure, which relies on the representation of basic operations suchas chemicals addition and solvent removal as movements on the phase diagram,for synthesizing separation process based on crystallization or precipitation.This procedure has been applied to synthesize separation processes for mixturesinvolving chiral compounds, solid solutions, fullerenes, amino acids, and proteins.The same idea can be applied to the separation and recovery of metal salts fromthe cathode materials. Two cathode materials, LiFePO4 and LiCoxMn1-xO2,are studied in this paper to illustrate how the SLE phase behavior can be usedto design the process and determine the optimal operating conditions of therecycling process. The general approach in utilizing SLE phase behavior to designthe recycling process and determine its operating conditions is discussed first,followed by using the two case studies to illustrate this general approach.

[1103]

A Drilling Scheduling Toolbox for Oil and Gas Reservoirs

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Drilling scheduling is a challenging task with considerable financial impacts, for which we develop a nonconvex MINLP formulation in this study. We consider the dynamics of the system and well as the economic forecasts and constrains. We develop a toolbox using genetic algorithm and an industrial reservoir simulator to solve this model. Our method provides detailed information for both short and long-term decisions. It determines the optimal drilling order, time and location, well types and hence the number of new injector and producer wells, and finally the production and injection flow rates. Our results indicate that we can decrease the rate of return (R.O.R) of an exploitation project by optimally scheduling the drilling activities.

[1154]

Superstructure-based optimization of biorefinery networks: Production of biodiesel

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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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Track 9.6. Environmental Systems Engineering

[13]

Process Simulation of Ammonia Recovery from Biogas Digestate by Air Stripping with Reduced Chemical Consumption

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Agriculture and the global society have growing interest in safe and environmentally sound manure handling systems. Sound manure handling is of great importance to reduce local and regional pollution such as odor emissions, nutrient leaching and eutrophication as well as greenhouse gas emissions on the global scale. Biogas treatment of manure is one way to recover resources by production of renewable energy and hence reduce GHG-emissions. Furthermore, odor emissions are reduced.

Biogas digestate also contains nitrogen (N) and phosphorus (P) of high fertilizer value. The N and P needs to be recovered to substitute inorganic fertilizers. In order to obtain a balanced fertilizer composition based on plant uptake and soil properties, separation of N and P is also of interest, where N can be recovered as ammonium sulfate by air stripping and subsequent acid absorption. P is mainly attributed to the solid fraction, where the N is mainly attributed to the liquid fraction.

The work presented will consist of process simulations by Aspen Plus of a plant treating the liquid fraction of biogas digestate at 90°C and recovers min. 95% N. The steady-state model uses an electrolyte-NRTL thermodynamic model to calculate the properties of the system, where a 12 stage stripper and a 5 stage absorber with sulfuric acid are the main unit operations.

Typically, the process is carried out at elevated pH by caustic addition, but the process presented here will be carried at pH 7.7 and the performance of the two systems is compared.

Additionally, the simulations will be optimized with respect to energy consumption as extensive heat recovery and air recycle are carried out. The process economy will also be evaluated with respect to capital costs, operational costs and product treatment costs.

[65]

Life Cycle Simulation for a Process Plant based on a Two-Dimensional Co-Simulation Approach

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The complexity of modern process plants is constantly increasing and thus the challenges for the engineering and operation of such plants. The use of simulations can be beneficial to investigate engineering and operations questions without the availability of the real plant. Today simulation is already utilized at particular steps within the life cycle of a process plant, for instance during the design phase. Later it is used for virtual commissioning to check out the automation system and for operator training. During the operation phase simulations can be used as assistance systems and for model based control. Even though the benefits of time and costs savings and increased quality are promising, it is not standard to use simulation as an integrated part of the plant life cycle. Reasons for this are in particular the effort for building up simulation models and that the decision to use simulation is not done on a life cycle perspective. Therefore the reuse of simulation models across the life cycle (horizontally) would be beneficial to foster a more integrated use of simulation.

Furthermore different simulation models can represent various parts of the plant. Looking at a controlled process plant there are components like the distributed control system (DCS), the signals and bus systems, the actuators and sensors and the process (with several sub-levels). To have a full virtual plant simulation, these levels must be also available within a simulation model. Thus the integration of different simulation models across these levels (vertically) is essential.

Another aspect is that simulation models can be realized in different tools. Thus the authors investigated the availability of co-simulation approaches to support a vertical and horizontal coupling of simulation models implemented in different tools. Basis for the valuation are requirements for co-simulation such as execution control, data exchange, configuration and management for simulations. The paper will present the results of a detailed evaluation of the Functional-Mock-Up-Interface (FMI), Cape-Open (CO), IEEE High-Level Architecture (HLA) and Open-Service-Gateway-Initiative (OSGI), for co-simulation needs. The results show that no approach currently fulfills all requirements for a horizontal and vertical coupling of simulation models. Cape-Open for instance is strong in coupling process models, shows however deficits at integrating dynamic models from other domains. Therefore the creation of a suitable co-simulation standard is suggested and a minimum implementation for a dynamic simulation control system (for e.g.: time synchronization, initializing, starting, running, pausing, stopping, snapshot triggering) and data exchange possibilities by using for instance an OPC or a Shared Memory interface are described. The work looks also at closing the gap between the design simulations focused on process modelling and simulations for virtual commissioning and operator training. An important aspect in this regard is for the example “real-time” capability of the co-simulation setup, as most automation system are running in predefined cycles and expect answers from the simulation system within these cycles.

Such a co-simulation standard would allow an integrated use of simulation along the plant life cycle with a maximum reuse of existing work. Furthermore in regards to modular plants and package unit integration this approach could also be the basis for simulation model integration as easy as the integration of a module into the real plant.

[164]

WWSD for distributed treatment of effluents

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Despite the technologies developed for water conservation inside an industrial plant some effluent streams still exist in the end of pipe. The distributed treatment of these effluent streams brings the opportunity to create wastewater treatments systems to accomplish with the environmental laws and in some cases contributes to water saving for the entire process. Wastewater Source Diagram (WWSD) is an algorithmic procedure for reducing the total wastewater treated flowrate by designing a distributed wastewater treatment system of effluents. Two criteria are taken into account for the synthesis of distributed treatment, the maximum concentration for discharge of contaminants and the treatment efficiency for contaminants. The WWSD procedure was applied to a real case to the treatment of effluents of the bioprocess laboratory. The effluents streams have one contaminant and multiple treatments with different removal rates are available for the synthesis of the wastewater treatment system. Although the distributed treatment achieves the lowest treated flowrate, the centralized system uses fewer units of treatment. Multiple scenarios for this mass exchange network are studied for this minimum treated flowrate but using different units of treatment. These treatments are compared by an economic evaluation carried for the centralized treatment and the distributed treatment of effluents.

[172]

Extending the benchmark simulation model no. 2 with processes for nitrous oxide production and side-stream nitrogen removal

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The Benchmark Simulation Model n°2 (BSM2) is a simulation environment built up with the aim of establishing a realistic reference where different plant-wide control strategies for wastewater treatment systems (WWTSs) can be tested and compared. As stated in Jeppsson *et al.* [1], there are many opportunities to extend this simulation model in terms of both mathematical models and of layout, which would allow the development and the evaluation of more specific control strategies. For instance, it is becoming more and more important for WWTS managers to reduce the emissions of nitrous oxide (N_2O), one of the most harmful greenhouse gases produced during the typical nitrogen removal processes. Another field where the development of control strategies is increasingly needed is in the side stream treatment unit where novel processes such as SHARON/Anammox treatment are increasingly adopted to improve plant treatment capability and to save operating costs. In this work, we expand the scope of the reference BSM2 implementation with the following two extensions: (a) the inclusion of N_2O production mechanisms by autotrophic and heterotrophic microorganisms in the mainstream activated sludge unit; and, (b) the addition of side-stream wastewater treatment technology to treat the effluent from the dewatering unit of the anaerobically digested sludge to reduce the nitrogen load recycled to the main wastewater treatment line. With regard to the inclusion of N_2O production, a calibrated and validated form of the Activated Sludge Model for Nitrogen by Guo and Vanrolleghem [2] including the production of N_2O by both denitrifying heterotrophs and ammonia-oxidizing bacteria was considered suitable in place of the Activated Sludge Model n°1 (ASM1). The main feature which needed to be revised while performing this expansion regarded the interface mapping the state variables used in the main stream model into those used in the model describing the anaerobic digestion of the sludge. With regard to spatial extension, the BSM2 layout is here extended by including a one-stage complete autotrophic nitrogen removal (CANR) process to treat the side stream originated from the dewatering unit. The process configuration and operation principles are detailed in Vangsgaard *et al.* [3]. The optimal value of the oxygen-to-nitrogen loading ratio used in Vangsgaard *et al.* [4] is used to assess a proper value for the oxygen mass transfer coefficient, which resulted to be 164 d^{-1}. The volume of the reaction is set up by iteration using a volumetric organic loading of 750 g $N.m^{-3}.d^{-1}$ which led to a volume of 400 m^3. Simulation results will be used to show how the aforementioned extensions impact the predictions of the whole plant. It will be demonstrated that the new plant-wide simulation model obtained from these extensions will provide a robust and realistic benchmark platform where control strategies for a large number of purposes can be designed and compared with one another.

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[183]

A Framework for the Dynamic Modelling of PI Curves in Microalgae

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Photosynthesis-Irradiance (PI) response curves constitute a powerful tool for characterizing the photosynthetic properties of microalgae. This paper presents a dynamic model capable of predicting the photosynthesis rate under dynamic light conditions. Fast and slow time-scale processes are coupled using fluorescence data for three different photoacclimation states. The model shows a very good agreement with the available experimental data and the values of the calibrated parameters are consistent with biological evidence. The predicted PI curves exhibit all the expected trends regarding their initial slopes, maximum photosynthesis rates, and photoinhibion effects. By analyzing the effect of different experimental protocols on the PI curve predictions, our results highlight the importance of an accurate description of the protocols used to obtain the experimental data.

[401]

Dynamic Ultrafiltration System Identification for Separation of Stable Emulsions

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The emulsions separation is one of the major processing challenges in the in the oil and gas recovery industry, so called produced water management. Produced water is the main liquid product after oil and gas extraction. This is a complex mixture of organic matter, oils, microorganisms, heavy metals, chemicals used for extraction, salts, dissolved oxygen, among others. The water treatment is challenging due to its dynamic characteristics which depend on the location, maturity of the well, extraction conditions and chemical treatments used for the oil/gas separation. Stable oil-water emulsions are generally separated using phase equilibria/specific gravity based technologies. It has been pointed out these technologies must be complemented by coalescence enhancers or chemical enhanced treatments in order to achieve the desired products quality for reuse or surface disposal. Forthcoming environmental legislations for water disposal will become stricter and it is in doubt that even optimal combination of conventional technologies can cope with the future challenges of produced water management. Encouraging results using membrane technology have shown its potential to achieve high performance separations required at industrial level. Membranes are attractive since they can deliver high selectivity and throughput, low chemical consumption, reasonable low energy consumption, compact modular design and use a simple regulatory control system. The main limitation using this technology is how to guarantee prolonged stable operation maintaining the effluent quality. This is due to two dynamically coupled phenomena referred to as concentration polarization and membrane fouling. To address this, dynamic operation of the system has been proposed using high frequency backshocks. The variant nature of the inlet water characteristics and dynamic operation of the system make that methodologies to determine sustainable flux (or critical flux) operation at field conditions require considerable experimental work.

To improve the methodologies, we propose to use modeling. Unfortunately, first principles models is unviable at this stage due to the lack of system understanding, especially the variant interactions between water, solutes and membrane as a function of the dynamic operating conditions. Even if possible, the obtained model will be valid only a narrow window making them unattractive. Therefore, the purpose of this work is to employ system identification methodologies in order to correlate the available information obtained during previous experiments. The available data sets cover the range of the operative window of interest, including different emulsion systems and operating conditions from subcritical to supracritical flux operation. If the statistical models results are satisfactory, they could be used in order to estimate the sustainable flux conditions from subsets of the experimental data. This task is not straight forward because the dynamic nature of the system. Thus, the tuning strategy can be improved.

The expected outcome of our efforts will be a better methodology to determine the sustainable flux operation of the dynamic membrane system, accounting for the dynamic interactions between the membranes and produced water. The obtained operational strategy could complement the obtained experimental insights in order to design full scale plants.

[429]

Progresses of PSE Studies on Water Networks and Industrial Application Practices in China

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As the water crisis is more and more serious, journal papers published on water networks have dramatically increased since about 2005. This work consisted of two parts. In the first part, an overview of the progresses of PSE studies on water network is described. In the second part, the industrial application approach with case studies in chemical enterprises is presented.

The documentation retrieval since 1994 is conducted. The topic is systematically reviewed in three levels according to the scale size: (1) water network integration and optimization in single enterprise, including Water Using Network (WUN), Wastewater Treatment Network (WWTN), Total Water Network (TWN), Complete Water Network (CWN） and Water Allocation and Heat Exchange Network (WAHEN) problems; Simultaneous process synthesis with heat and water integrations are also included; (2) inter-plant multiple water network integration including water network integration in eco-industrial parks; (3) virtual water and water footprints studies across prefectures /countries. These studies are very useful in water conservation, wastewater reduction, energy efficiency improvement in enterprises and eco-industrial parks, and also provide the basis for policy arrangements for governments particularly those of water scarce areas.

The industrial implementation approach called "Three Steps Approach" is created in China. The three steps are: (1) enterprise-wide water balance test and measurement; (2) water system integration and optimization calculations and the enterprise-wide water system decomposed into seven subsystems which are improved correspondingly. They are: freshwater treatment system; water transport pipeline system; process water-use system; cooling water system; desalination water system; living water system; wastewater system; (3) wastewater regeneration and reuse after wastewater reduction. According to our experience of more than 20 petrochemical and coal chemical enterprise projects, 20% to 60% amount of freshwater could be saved with this approach. A successful case study showing the example of implementation approach application is presented in detail.

[452]

Multi-objective Optimization of Small-size Wastewater Treatment Plants Operation

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This paper deals with the multi-objective optimal control of small-size wastewater treatment plants. Such plants consist currently of a single alternately aerated activated sludge reactor where suspended microorganisms degrade the incoming pollution, and a settler in which the sludge is separated from the treated effluent. The underlying biochemical and physical separation phenomena are modeled using the well-known Activated Sludge Model N°1 and Takács models respectively. In-situ incineration of the extracted sludge for electricity production is investigated as a promising option to reduce the operating costs. Two objective functions to minimize are considered, the process exploitation costs and the nitrogen discharge. The goal of this work is to determine the Pareto front characterizing the trade-offs between the treatment quality and operating costs. Two situations are considered: in the first, sludge is dried then incinerated, while in the second, sludge disposal and valorization are not accounted for. The problems are solved using an elitist multi-objective genetic algorithm.

Compared to the literature, emphasis is put on a proper formulation of the optimization problem so as to get physically relevant solutions. Hence, a large time horizon of 100 days is considered in order to guarantee that the computed optimal operating strategies ensure a sustainable plant functioning. Discharge constraints are taken into consideration only after 86 days: such a large time delay ensures that the cyclic steady state is reached. Indeed, activating a constraint during the transient step makes the computed solutions depending on the - arbitrarily - chosen plant's initial state (of which effects should vanish with time). Solids retention time is constrained between 4 and 30 days in order to guarantee flocs settleability and to limit sludge mineralization. The reduction of the oxygen transfer rate depending on the suspended solids concentration in the mixed liquor is also included in the model. Finally, the average dissolved oxygen concentration during each aeration/non-aeration cycle is constrained to be higher than 2 g.m-3 (aerobic conditions) or lower than 0.1 g.m-3 (anoxic conditions). Indeed, preliminary tests demonstrated that such constraints are necessary to maintain the optimal solutions within the limits of validity of the mathematical model.

The computed Pareto fronts provide a clear picture about the interdependencies between the treatment's quality and exploitation cost. Such data help engineers in judging the trade-offs between the set of optimal solutions, and hence, choosing the most suitable operating strategy. Sludge incineration has been shown to be quite profitable energetically, especially when high nitrogen discharge is tolerated. However, this sludge valorization option does not allow attaining the plant's electrical autonomy.

[464]

Pipeline Merging Considerations for the Synthesis and Design of Interplant Water Networks with Wastewater Treatment, Regeneration and Reuse

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The development of effective wastewater regeneration and reuse networks has been a prominent research focus, in response to the growing demand for high-quality freshwater supplies by the industrial sector. However, many naturally-existing water reserves suffer from the inability to be consistently replenished. Hence, increased rates of freshwater consumption places excessive pressure on existing water resources since many of which are unable to sustainably satisfy the increased industrial water consumption requirements. As a result, industrialized regions are recognizing the benefits of promoting effective wastewater treatment, regeneration and reuse strategies as a means of supplementing the use of freshwater reserves.

Much of the research attention so far has primarily involved identifying optimal wastewater treatment and reuse strategies, in which several wastewater-producing operations are matched with a number of water-consuming operations, and/or assigned to undergo a series of treatment steps before reuse, if necessary. Moreover, a single pipeline is designated for every viable water allocation identified. This has been consistently observed in many of the previous research contributions that involve interplant water network synthesis. In an attempt to enhance the water network design process, several representations that account for a number of pipeline merging scenarios have been investigated for wastewater reuse networks [1]. This work is an extension to our previous contribution, which incorporates options for the synthesis and design of merged pipeline networks involving wastewater treatment, regeneration, and reuse. In addition to the improved ability of screening of less complex pipeline networks, merging together common pipe segments that carry similar water qualities have been found to allow for various cost-enhancements in the designs obtained. In order to avoid unwanted water mixing in the merging procedure, the proposed methodology can be carried out on pipelines that carry treated, and untreated water qualities, individually. Additionally, extra pipeline assembling opportunities have been identified to exist for centralized treatment facilities, in contrast to the de-central treatment options.

As an illustration, an artificial case study has been implemented, involving a number of water-consuming and wastewater producing processes. Moreover, a number of centralized and decentralized wastewater treatment options were also incorporated. The study accounts for spatially constrained water transport, since the various plant arrangements, and common available infrastructure were all incorporated into the study. The results indicate very attractive wastewater treatment and reuse schemes for the water network designs extracted. Moreover, several cost-efficient water networks that involve many merged pipeline segments in the designs extracted, have been identified.

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Simultaneous Design and Planning of CO2 Transport Pipeline Network for Carbon Dioxide Capture and Sequestration Project

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Carbon dioxide (CO2) capture and sequestration (CCS) can significantly reduce emissions from large stationary sources of CO2, which include coal- and natural-gas-fired power plants, as well as petro-chemical plants. CCS is a three-step process that includes: capture, compression and transportation (usually in pipelines), and injection and sequestration. The capital investment and operating cost of the pipeline network have a direct impact on the success or failure of a CCS project.

The planning, scheduling or design of pipeline systems have been studied by many researchers in the literature1-2. Up to now, only a few works have addressed the synthesis and design problem for CO2 transport pipeline network3. But most of them do not consider the influence of strategic planning in the design procedure of network and pipeline. In previous sequential frameworks, the planning is optimized for the predefined pipeline network, or vice versa.

In this paper, a superstructure-based MINLP approach for simultaneous design and planning of CO2 transport pipeline network targeting on minimizing the overall cost in a CCS project is presented. Different from the former study, the whole problem is reformulated in a framework of supply chain. Each industrial plant is regarded as a supplier, who provides CO2 raw material at its own capture cost. Each big pump station is regarded as the factory and each sequestration side is regarded as a customer, who wants to buy CO2 product at the price of its own sequestration revenue (mainly comes from government subsidy). The main features of this approach are listed below:
1. The diverse CO2 capture and sequestration capacities and costs in different sources and sinks are considered. Their change trends in the horizon are also included in the model. So the network nodes and transporting amounts of CO2 are optimization variables rather than predefined parameters.
2. Supplier-intermediate site-customer and supplier-supplier connections are introduced in the network superstructure to achieve the sharing mechanism of pipelines in the long distance transportation, which leads to considerable expense reduction.
3. Simultaneous optimization of the planning, network structure and the diameter of each pipeline in the framework of supply chain.

Finally, the potential of the proposed method is demonstrated using a simplified real-life CCS project in north China.

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[471]

Environmental, Societal and Economical optimization of a bioethanol supply chain

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The objective of this contribution is to present a mathematical model (Mixed Integer Linear Programming) for the facilities and biorefinery locations, and the logistic management. For the model formulation, we first need a geographical discretization of the region in which the supply chain would be implemented and the identification of the different biomass sources and their availability in this region. The technological, ecological, economic and social data are also mandatory to run the model. As in supply chain there are short-term and mid-term decisions, the time horizon must be discretised. The original contents of the model are threefold: integration of multiscale aspects, taking into account of the biomass characteristics, optimization of the supply chain with economic, environmental and social criteria. As a result the model determines the number, the location and the capacity of bio refinery and facilities.

[565]

Operation optimization of ammonia nitrogen removal process in coking wastewater treatment

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One of the key steps of coking wastewater treatment is ammonia nitrogen removal. It is normally realized by a process combining distillation operation with bio-treatment, in which the high cost distillation is designed to reduce ammonia nitrogen low enough for the following low cost bio-treatment. Many efforts have being done to optimize the structure and operating parameters of these two units. However, to the authors' best knowledge, little work has been done considering the interaction between units. Obviously, it needs to make a balance between these two units operation in order to reduce the operating cost. In this paper, a mathematical model of the overall ammonia-nitrogen removal process, which combines distillation with shortcut nitrification/ANAMMOX/denitrification (O1-A-O2), is proposed for its operation and structural optimization. The proposed model is formulated as a mixed integer nonlinear programing (MINLP) problem with aim of minimizing operating cost. The main decisions include determining ammonia-nitrogen outlet concentration, reaction recycle time and passby flowrate of O1 reactor subject to compliance with the maximum allowable inlet ammonia-nitrogen concentration limits of the bio-treatment and discharge regulations. We also develop shortcut models for the ammonia distillation operation and bio-treatment process based on rigorous model calculation data and theoretical analysis to enforce solution convergence. Computational studies are carried out via GAMS/DICOPT using industrial operating parameters of the typical coking wastewater treatment system as input. The results indicate that the minimum operating cost is obtained at ammonia-nitrogen outlet concentration 128 mg/L, reaction recycle time of O1 10 h and passby flowrate 11.448 m3/h when the ammonia-nitrogen inlet concentration of distillation column is 4 000 mg/L. In our following work, we will incorporate tight bounds on the variables and more constraints that enforce certain operation and design specifications in order to more effectively solve the MINLP model to global optimality.

[567]

Systematic Design of High Performance Post-Combustion CO2 capture Flowsheets Considering Different Solvents

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Solvent-based chemical absorption/desorption systems are the most mature among industrial CO2 capture applications because the technology is well established and the process can be easily retrofitted onto existing plants. Despite this maturity, a major challenge hindering their widespread adoption in industry is the very high cost introduced to the operation of CO2 emitting plants. Modifications on the conventional absorption-stripping loop used in solvent-based post-combustion CO2 capture processes have so far shown a positive impact on the overall efficiency and cost of the process. These modifications are classified as either structural, mainly focusing on the redistribution of the material and energy flows to the separation columns, or operational, referring to the conditions imposed on the unit operations to meet the design specifications. The selection of the solvent used for the chemical absorption is usually associated with the need for increased CO2 capture capacity as well as the low energy demand for regeneration in the desorption column.

This work focuses on the development and evaluation of several combinations of amine solvents and innovative flowsheet structures for the efficient separation of CO2 from a flue gas stream. The proposed flowsheets are generated using a generalized design framework which incorporates a robust and compact modeling scheme in the context of a flexible and inclusive synthesis model. The framework serves as a mathematical tool able to reproduce any potentially favorable representation of solvent based CO2 capture processes supported by an underlying superstructure. The superstructure consists of modules representing generic process tasks (e.g., reactive and nonreactive separation, heat transfer, mixing) and interconnecting streams emulating material flows. The behavior of the separation columns in the process is described using an equilibrium based (EQ) model, combined with orthogonal collocation on finite elements approximation techniques (OCFE). EQ/OCFE model formulation enables a robust and flexible representation that accommodates high resolution in describing the occurring phenomena in a compact form. The proposed flowsheet configurations are chosen aiming at the overall enhancement of the main driving forces in the separation columns and thus, the intensification of the process itself. Flowsheet designs including different stream topologies, heat redistribution through suitably incorporated heat injection/removal modules and cascades of desorption columns, to name but a few, are among the investigated options.

All proposed developments are implemented in the optimal design of a CO2 capture process characteristic for quicklime or cement plants. Such plants rank amongst the highest industrial CO2 emitters due to the combined generation of CO2 in the calcination and fuel combustion steps. A number of commercial candidate solvents, namely monoethanolamine (MEA), diethanolamine (DEA) and 2-amino-2-methyl-1-propanol (AMP) have been tested. The thermodynamic behavior of the CO2-water-amine mixtures is described through pressure-loading relationships extracted from the Statistical Associating Fluid Theory for potentials of variable range (SAFT-VR). Opportunities for significant structural and operating improvements result from the evaluation of numerous flowsheet-solvent combinations.

[682]

Solubility measurement and process simulation of CO2/CH4 gas mixtures using Ionic Liquids

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Ionic Liquids (ILs), with the character of low heat capacity and corrosive, nonvolatile and good CO2 solubility, in particulate preferred to a high CO2 partial pressure, which could be used as additive to save CO2 regeneration energy from utilize biogas on a large scale and commercialization. Pure ILs have been studied several years for CO2 capture, however, biogas upgrading by ILs are quite few, in particulate organic solvent-ILs mixtures. In this work, organic solvent-ILs mixtures was developed as physical absorbents for biogas upgrading process, and the separation performance by experiments and simulation was evaluated. The solubility of CO2 and CH4 in the absorbent was measured using a vapor-liquid equilibrium apparatus to provide necessary parameters for process simulation, and evaluate the CO2/CH4 selectivity, absorption rate and capacity. The physical properties of ILs were estimated by FCCS model, and PR equation of state was adopted for designing the thermodynamic models of VLE of capture system and the parameters were regressed based on the experimental data. The predicted values from the thermodynamic models are in good agreement with the experimental results.

The biogas upgrading systems using pure IL, organic solvent and organic-ILs mixtures were assessed in terms of their energy consumption and environmental impacts, while taking CH4 recovery ratio, specific energy consumption, energy efficiency and Green Degree as assessment indicators. The results showed that organic-ILs mixtures systems required lower energy demand than other systems, and also produced lower environmental impacts. All these results in this work demonstrate that organic-ILs mixture is a promising solvent for biogas upgrading technologies.

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[749]

Evaluation of Qualitative Trend Analysis as a Tool for Automation

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Qualitative Trend Analysis (QTA) comprises a diverse set of algorithms for time series analysis in view of process diagnosis [1] and data mining [2]. QTA based automation of a batch process is not evaluated yet [3]. Biological wastewater treatment plant automation with QTA is proposed here.

The studied wastewater treatment plant Hard in Winterthur (Switzerland) has three aerated tanks for biological oxidation between the primary clarified and the secondary clarifier. The difference between a pH measurement in the first aerated tank (upstream, us) and the last aerated tank (downstream, ds) is registered. An ammonium (NH_4^+-N) ion selective electrode (ISE) is used as a reference.

The maxima in the ammonia and pH difference signals are remarkably synchronous. Our control scheme relies on the minima and maxima in the pH difference signal. The recognition of pH minima and maxima is based on the Qualitative State Estimation (QSE) algorithm. Similarly to Qualitative Path Estimation (QPE), it is based on kernel regression and a Hidden Markov Model (HMM) [4-5]. By means of the QSE algorithm one can identify whether the monitored system is experiencing a high or low ammonia load. The proposed control system adjusts the setpoints for the oxygen concentration accordingly.

Acknowledgments

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[892]

A detailed mathematical modelling representation of clean water treatment plants

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One of the biggest operational risks to water companies arises from their ability to control the day to day management and optimisation of their water treatment systems. With ever increasing pressures to remain competitive within the global market, companies are looking for solutions to be able to make predictions on how their chosen treatment processes can be improved.

Most modelling work within water operations has so far been based on empirical observations or hydraulic modelling rather than on fundamental mathematical descriptions of the process which is the focus of this work. Mathematical models are essential in order to describe, predict and control the complicated interactions between the different parts of the treatment process, a concept which is well understood within the process industry but not yet established within the water treatment industry. Accurate description of water treatment may, however, result in highly complex models, which may not be very useful from a practical, operational point of view, hence this work will also consider the level of modelling detail required to accurately represent a water treatment plant.

The main objective of this work is the consideration of a complete mathematical model of an entire water treatment plant which enables a wider view on how changes in one processing unit will affect the treatment process as a whole. The processes used for potable water treatment plants can vary dependant on the source of water and water quality, but this work focuses on a 'conventional' water treatment process which utilises coagulation and flocculation, sedimentation, filtration, and chemical disinfection. The performance of the process models are first verified individually and are then combined to enable the simulation of a complete water treatment work.

It will be shown that our model is able to predict for instance how the flow rate of water into a sedimentation unit affects the formation of the sludge blanket, as the sludge blanket can be broken if the flow rate is too high, and not form if the flow rate is too low. If the sludge is broken, or not formed then the supernatant, which is the clear water above the blanket, flowing into the following unit will be of poor quality as an increased amount of flocs are allowed to move forward. It will also be shown that the overall model can predict how for instance a change in the coagulant dose will affect the water quality further downstream. Our work demonstrates for the first time how complete model prediction in a water treatment plant can improve operation and reduce operational risk.

[900]

Modeling rate enhancement of carbon dioxide absorption in chemical solvents using carbonic anhydrase enzymes as promoter

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One of the largest obstacles today's society faces is to provide safe and reliable energy sources, while reducing carbon dioxide emissions. Post combustion carbon capture technology is capable of resolving these two issues in the near future. Until the regenerative technologies are mature enough to provide energy for the whole population, carbon dioxide emitted by fossil fuel burning power plants can be captured and stored beneath the surface.

In this process technology a liquid solvent is cycled continuously between the absorber and desorber. In the absorber CO2 is captured from the exhaust gas at a moderate temperature and it is released in the desorber under the input of thermal energy. The driving force for this process is the difference between the partial pressure of CO2 in the gas phase and its corresponding thermodynamic CO2 solubility in the solvent. As the process is performed at almost ambient pressure the partial pressure of CO2 in the exhaust gas of a power plant is rather low, and places high requirements on the absorption process. For this purpose a chemical absorption process is chosen where the solvent reacts with the physically bound CO2. The decrease of CO2 in the liquid bulk leads to an increased diffusion of CO2 from the gas interface and therefore enhances the absorption. The rate of chemical absorption is dependent on the reaction rate between the solvent and CO2 and also the diffusion of all the involved compounds.

In this study the application of the enzyme Carbonic Anhydrase as a kinetic promoter on chemical solvents are investigated. This enzyme catalyzes the reaction between CO2(aq) and HCO3-, and enhances the CO2 reaction without interfering with the solvent reactions.

Experiments on the rate of absorption are carried out in a gas liquid contactor with different chemical solvents with and without enzymes. A mathematical model will is created which can describe the rate of CO2 absorption into the solvents coupling the chemical reaction and diffusion, with emphasis to explain the absorption rate enhancement with enzymes.

[914]

Water resources management with dynamic optimization strategies and integrated models of lakes and artificial wetlands

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The wastewater treatment plants allow improving water quality, by removing contaminants from human and industrial activities, which implies a reduction in environmental pollution. Due to this, an adequate design of networks for wastewater depuration is fundamental, as well as their optimization which nowadays should be focused on sustainability factors, such as worker stress, work satisfaction and attitudes to achieving sustainability. Those are, social indicators which should be considered together with the environmental and economic dimensions of sustainability. In this work a flexible methodology that adapts to the needs of treatment is proposed, that is, the choice of the different elements of the process depends on specific goals, wich are related to multi-criteria based problems such as effluent quality, sludge reuse, energy efficiency and cost. Furthermore, we start off the supposition that some of the parameters are uncertain and variable, allowing the plant design to be robust and flexible and the optimization problem to be flexible from a mathematical point of view.

The methodology we propose is based on the generation, evaluation and selection of configurations and methods (physical, chemical and/or biological) for the different stages of treatment, in terms of chemical and biochemical oxigen demand, the amount of total suspended solids and heavy metals, among other variables that have to stay within limits of sustainable metrics. For example, let us consider one of the methods of treatment most widely used; this is the activated sludge process, which mainly consists in five stages: preliminary, primary, secondary, tertiary and sludge treatment. There is a wide range of different plant and networks configurations and big design space which have to be evaluated and debugged in order to screen out infeasible designs and select the suitable one. In this work, we present a methodology to address this.

[974]

Design and optimization of sustainable wastewater treatment plants networks

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The wastewater treatment plants allow improving water quality, by removing contaminants from human and industrial activities, which implies a reduction in environmental pollution. Due to this, an adequate design of networks for wastewater depuration is fundamental, as well as their optimization which nowadays should be focused on sustainability factors, such as worker stress, work satisfaction and attitudes to achieving sustainability. Those are, social indicators which should be considered together with the environmental and economic dimensions of sustainability. In this work a flexible methodology that adapts to the needs of treatment is proposed, that is, the choice of the different elements of the process depends on specific goals, wich are related to multi-criteria based problems such as effluent quality, sludge reuse, energy efficiency and cost. Furthermore, we start off the supposition that some of the parameters are uncertain and variable, allowing the plant design to be robust and flexible and the optimization problem to be flexible from a mathematical point of view.

The methodology we propose is based on the generation, evaluation and selection of configurations and methods (physical, chemical and/or biological) for the different stages of treatment, in terms of chemical and biochemical oxigen demand, the amount of total suspended solids and heavy metals, among other variables that have to stay within limits of sustainable metrics. For example, let us consider one of the methods of treatment most widely used; this is the activated sludge process, which mainly consists in five stages: preliminary, primary, secondary, tertiary and sludge treatment. There is a wide range of different plant and networks configurations and big design space which have to be evaluated and debugged in order to screen out infeasible designs and select the suitable one. In this work, we present a methodology to address this.

[1009]

Life Cycle Assessment Studies of Chemical and Biochemical Processes through the new LCSoft Software-tool

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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 decision making of selecting the preferable product or process from different alternatives. For more sustainable process designs, technical requirements have to be evaluated together with environmental and economic aspects. In our research group, the LCSoft software-tool has been developed to perform LCA with ability to be integrated with other process design tools such as process simulation, economic analysis (ECON), and sustainable process design (SustainPro). Continuing on the development of LCSoft, this research focuses on improving the program in three main parts. The first task has been to extend Life Cycle Inventory (LCI) database while the second task has been to perform uncertainty analysis function in order to investigate the influence of uncertainty in LCI to the assessment results. The third task deals with validation and improvement of LCSoft by testing it against several case studies and comparing the assessment results with other available tools. The results show the improvement in the performance of LCSoft on various applications, giving accurate and reliable results. Furthermore, LCSoft can support the user to achieve the targeted design effectively since it is integrated with economic analysis and sustainable process design tools.

[1043]

Control Structure Design of an Innovative Enhanced Biological Nutrient Recovery Activated Sludge System Coupled with a Photobioreactor

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Conventionally, the objective of wastewater treatment is the elimination of organic and inorganic pollutants. Current research promotes a paradigm shift, whereby wastewater is not only considered as a source of pollution but also as resource of energy, nutrients and water. The TRENS system is a train of biological units designed for resource recovery from wastewater. It is a sequence consisting of an enhanced biological phosphorus removal and recovery system (EBP2R) coupled with a photobioreactor (PhBR). The purpose of the EBP2R system is to produce an optimal culture medium for the downstream algae cultivation [1]. In this work, we apply a systematic strategy to develop a control structure to ensure an optimal nutrient balance to feed to the PhBR, so the grown microalgae suspension is suitable for fertigation (irrigation and fertilization of agricultural crops). To this end, we follow the plantwide stepwise procedure proposed by Larsson and Skogestad [2]. First we define the goals of the system. The primary goal is to achieve a high phosphorus (P) recovery rate. The EBP2R was previously optimized through scenario simulations and it was found to be able to recover up to 75% of the influent P load [1]. The secondary objective is the optimal algal cultivation by providing an optimal nitrogen-to-phosphorus molar ratio (N-to-P ratio) to the PhBR. In this case study we consider the cultivation of a mixed green microalgae culture which optimal N-to-P ratio is 16 [3]. Then, a regulatory control layer is proposed based on process knowledge. This layer is composed of 4 different feedback control loops. Oxygen level is controlled through kLa manipulation, the P and N loads are controlled through the flow rate of the two effluent streams of the EBP2R and the solid retention time is kept through wastage of sludge from the bottom of the secondary clarifier. The pairing of variables is double-checked with the relative gain array, which shows that the interaction between the proposed control loops is minimal. Afterwards, the system is tested under different scenarios, where the influent quality is disturbed following a step change. The control system is able to reject most of the disturbances successfully. However, when the P-recovery capacity is limited by the influent P, the control system is not able to keep the set point for P load. Nevertheless, the maximum percentage recovery from the influent P is kept. In this scenario, the N-to-P ratio is still optimal, so the algae are able to take up all the incoming nutrients into the PhBR. In a final step, the performance of the control structure is assessed through dynamic simulations. The complete study, including the different scenario simulations, will be presented in the full paper.

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Maria-Ona Bertran, Thomas Bisgaard and Rebecca Frauzem (Eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. 31 May - 4 June 2015, Copenhagen, Denmark

Track R. Renenseng EU Project

[249]

Production of phthalic anhydride from biorenewables: process design

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The renewable production of chemicals has recently attracted an increasing attention. In fact, the co-production of value-added products along with biofuels would enable biorefineries to explore cost-effective solutions to meet environmental goals, answer the energy security and climate change concerns [1].

Biotechnology and chemistry has shown the tremendous potential of biomass to produce bulk and niche chemicals. Several attempts have been made to select the most promising conversion routes [1, 2]. In the biorefining context, Process System Engineering methods have been mainly focusing on biofuel process and supply chain modelling and optimisation [3, 4]. Some works have dealt with optimisation frameworks based on technological superstructures to screen promising biomass conversion pathways [5]. Only a limited number of studies have proposed rigorous techno-economic assessments of selected bio-based chemicals [6]: process intensification has proven to be essential to cut the production costs.

Phthalic anhydride is a chemical of key importance in the production of plasticizers, polyesters, and resins. Its production (currently about 3Mt pa) is based on fossil feedstocks, as such its market would be affected by petroleum depletion concerns. A renewable route to phthalic anhydride has been recently discovered [7] using biomass-derived furan and maleic anhydride. Techno-economic analyses of this process are required to assess its actual scalability.

In this work, a conceptual design of the production process of phthalic anhydride from corn stover is proposed. The study was carried out in Aspen Plus® and was based on an extensive survey of technical chemistry solutions (i.e. experimental and industrial) to screen promising process configuration alternatives. Opportunities for process intensification and energy optimisation were investigated. The techno-economic assessment of the process based on rigorous mass and energy balances has revealed that only developing a full biorefinery with multiple secondary products along with the main one would make the business profitable. Sensitivity analyses were carried out on relevant factors (e.g. product prices, consumables cost) to study the effects on the flowsheet configurations and the product portfolio.

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[265]

Sustainable Process Design under uncertainty analysis: targeting environmental indicators

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The synthesis and design of sustainable chemical processes poses a complex decision-making problem that aims to minimize the external resources consumption and the respective environmental impact while maximizing the economic profitability. This problem can be addressed through mathematical programming using a multi-objective optimization framework. Nonetheless, the main limitation of this method is the amount of data required and the uncertainties to which they are subject to. Among others, these uncertainties may include market price fluctuations, manufacturing/technical performance variations and environmental model predictions. How to systematically identify and manage the sources of uncertainty and how to quantify the impact of those in the system sets the objective for this contribution.

A considerable number of approaches have been proposed in the literature for this class of problems; however, coupling environmental with economic sustainability metrics, both under uncertainty, remains a big challenge that has not been comprehensively addressed. In this study, we propose the implementation of a multi-objective multi-criteria optimization approach based on stochastic mixed-integer nonlinear programming with comprehensive uncertainty analysis. For the implementation, a Computer-Aided Framework for Sustainable Process Design with particular emphasizes on early stage alternative generation and evaluation is developed.

For the uncertainty analysis, the engineering standard Monte Carlo technique is used (Sin et al 2009), which comprises the following steps (i) the identification of uncertainties in evaluation data and characterization of uncertainties using appropriate statistical distributions, and, (ii) the sampling from uncertainty domain using Latin Hypercube Sampling (LHS) and(iii) formulation and solution of optimization problem both for mapping input uncertainties as well as sample average approximation

In order to highlight the main features of the methodology, namely the impact of uncertainties in economic and environmental indicators on sustainable process design, and to understand how they propagate and affect the decision-making procedure, a biorefinery case study from the edible oil industry is formulated and solved. The optimal processing design under uncertainty is obtained for the conversion of glycerol, co-product of biodiesel plants, to produce a set of value-added products that are usually delivered by the petro-chemical industry.

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[719]

Model Integration Using Ontology Input-Output Matching

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Model integration is a process that aims to amalgamate models and facilitate their sustainable use in operation. The only existing model integration framework is the CAPE-OPEN, proposed by the European Process Industries which established a software based interface, Common Object Request Broker Architecture (CORBA). More precisely, CORBA provides a Common Interface Bus that allows individual models to reside in multiple computer systems and communicate with each other. Whilst the CAPE-OPEN standard is a widely recognised standard, a disadvantage has been identified in the lack of flexibility in input/output (I/O) architecture.

In this paper we propose ontology controlled model integration, which builds upon the existing CAPE-OPEN framework and replaces the CORBA object bus with more flexible semantic Repository, as shown in Figure 1. The whole process is controlled by the domain ontology which models the model/simulator functionality in relation to process requirements. Process models themselves are treated as services. Each model is semantically described using Ontology Web Service Description (OWL-S) framework, registered as the instance of the domain ontology and published in the purposely built public repository for input/output matching with other available models. The particular role of the domain ontology is to enable model registration and a full semantic description of its input(s), output(s) and environment requirements. On the other side, the particular role of OWL-S ontology is to enable all stages of model integration; i) model discovery (in public repository(ies)), ii) model selection (screening of all possible options which satisfy requestor functionality, iii) model composition to respond the requestor functionality, and iv) model execution. The model selection and model composition stages are performed by semantic input/output matching[1] which allows for partial matching and hence for a high degree of flexibility in model integration. It is also important to mention that along with the model composition and integration the proposed framework allows for integration of data residing in various forms of databases and concomitantly semantically described in the same way models.

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[804]

Life cycle assessment of biorefinery products based on different allocation approaches

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Biorefineries constitute representative examples of multifunctional systems which are able to produce,similarly to conventional petroleum refineries, a wide range of chemicals(pharmaceutical constituents, plastics, food additives etc.), energy carriersand power through the optimal use of diverse biomass forms (wheat straw, oils,wood chips, municipal solid waste). For this purpose, biorefineries typicallycomprise a complicated, integrated network of physical and chemicaltransformation processes, such as mechanical and physical biomass pretreatment,pyrolysis, gasification, catalytic and enzymatic reactions, and downstreampurification processes. For the environmental sustainability assessment of these complicated production systems, Life Cycle Analysis (LCA, ISO-Norm 14040)is considered as a widely acceptable methodology from scientists and engineers including,however, the debated aspect of partitioning the impacts among the co-products' inthe biorefinery product portfolio.The aim of this study is to present theinfluence of the various allocation approaches on the LCA results ofbiorefinery products. The framework of this analysis systematically incorporatesthe steps of the LCA methodology as described in the ISO norms and estimatesthe impacts related with the products of interest, taking into account thecontribution of the co- and by-products in the overall production path. Forthis reason, two wider approaches were adopted, the attributional whichdescribes the impact of the production process itself from a retrospectivepoint of view, and the consequential which focuses on the changes in the levelof the output (as well as consumption and disposal) of a product, including market effects fromincreasing or decreasing demand for the study product, having therefore a more prospective point of view. Several scenarios which describe the possible options for handling those products, were developed and assessedbased on different allocation methodologies, namely system expansion (substitution method) and partitioning methods according to the mass, thermal and economic values of the co-products.To perform the LCA, a detailedgate-to-gate inventory analysis for the study systems was undertaken including material and energy flows, and discharges in air, water and soil. Data for mass and energy balances were gathered from literature references and pilot plants that provide detailed information about the process flowsheets (quality of rawmaterial, specific design characteristics, energy/cooling demand etc.). In addition to detailed process information, the use of existing life cycle databases (e.g., Ecoinvent database, versions 2.2 and 3) and tools (e.g.,Simapro 8.0.2) was necessary. The estimation of the life cycle impacts of the processes was performed using the Global Warming Potential (GWP), CumulativeEnergy Demand (CED) and RECIPE methodologies which provide an assessment of the burdens through the associated LCA indicators.The outcome of this approach is to provide a range of LCA metrics emphasizing at the variation of the results accordingto the followed allocation methods and to identify those propertiesof products (physical, economic, thermal) and system factors (processes to besubstituted from the renewable ones, degree of utilization of co- and by-products from the markets etc.) which dominate the LCA results.

[1136]

Optimization of multiphase reactor systems: Impact of different mass transfer correlations on the real design of bio-reactors

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The ultimate aim of chemical process design is to synthesize a process that enables the production of desired fuels and chemicals in the most cost effective and environmentally benign manner. This is also the goal of the emerging biorefinery design. For the fractionation of biomass and its conversion to products, new chemistries are recently developed or are still under research. The design of the bioreactors is mainly based on experience and heuristics developed for conventional reactors. Bioreactors are mainly heterogeneous systems, strongly non-ideal, whose thermodynamic correlations are difficult to extract. Heterogeneous reaction systems imply the necessity for the determination of supplementary factors, which are introduced into the corresponding mathematical models. In contrast with the homogeneous case, in the heterogeneous schemes, apart from the kinetics and the heat transfer effects, the mass transfer and the general hydrodynamic behavior of the system has to be determined. The overall reaction rate depends on kinetics and on the system's ability to exchange mass between different phases. Consequently, the need for determination of the necessary mass transfer and hydrodynamic coefficients cannot be avoided. This work presents a superstructure-based simulated annealing approach to the synthesis of reactor networks in an equation-oriented environment. The problem under consideration entails the optimization of a superstructure of ideal reactor units involving CSTRs and PFRs with feed distribution options as proposed by Kokossis and Floudas (1990). Hydrodynamic and mass transfer correlations are introduced into the mathematical model of the optimization problem for different real reactor designs. The main target is the investigation is the impact of these correlations to the final design decision of biochemistries recently developed for their implementation in biorefineries. The appreciation of different, competitive equations and their final selection is dominated by their operability, as far as the optimization process and the corresponding mathematical programming are concerned. The importance of the proposed correlations, not only of the objective function itself, but also in other parameters, such as the reactor type and volume will be based on the final results obtained from the optimization model.

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Late Additions

[498]

Key Performance Indicators for Monitoring and Evaluation of PID and APC Strategies at Manufacturing Operations Management Level in a Natural Gas Processing Unit

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Monitoring and control of proper Key Performance Indicators of plant performance have high correlation with business performance. Thus it is very important at plant-wide level to ensure that process control developments are being made aligned with business strategy, since Advanced Process Control projects have as ultimate goal to help achieving gains in this direction. The ISO 22400 "Key Performance Indicators (KPIs) for Manufacturing Operations Management" is an international standard currently under development. This new standard defines KPI as quantifiable level of achieving a critical objective derived from measurements, data and/or other key performance indicators. Performance parameters for assessment of PID and multivariable controllers have been discussed in literature but they don't translate the loop performance into manufacturing operations level concepts. The Stabilizer Tower is responsible for removing light components of crude oil that reaches the tabs and desalt tanks at the entrance of the plant. The operation of this column aims to ensure low Reid Vapour Pressure in stabilized oil output stream, thus decreasing its flammability and avoiding the formation of gas during storage, while maximizing oil production. Due to the large number of production wells and its various operating conditions, the inlet of the plant presents high variability in terms of flow rate, composition, temperature and pressure throughout the day. In this scenario, the traditional PID control strategy does not show satisfactory performance in temperature control of the stabilization tower. The instability of this tower leads to problems for downstream processes (as NGPUs), interfering with the profitability of the plant and the storage conditions. In this work, the advanced control strategy applied in Tower Stabilization Unit is developed and KPI for manual, PID and APC operations are determined. The advanced control employed is based on the type Predictive Process Models. Dynamic models considering supply disruptions in the tower and process response were identified. The implementation aimed to promote a low temperature variability tower, stabilizing the supply of NGPU. The predictive controller action employee can be seen in correct anticipation of control actions to prevent disturbance input promote future impact on the process conditions. It was verified that the predictive control action was effective even in extreme conditions such as PIG. These performance gains are mapped to plants KPI indexes. This paper is about selecting and using PID and APC Key Performance Indicators to help performance evaluation and comparison at plant-wide level. In this work we explain what KPI are suitable to use and their illustration of the impact of the new control strategies in the plant through an example of how they have been implemented in an industrial Oil and Gas Processing Unit.

[959]

Self-adjusting Soft-Sensor Development and Implementation for Monitoring of LPG Quality in a Debutanizer Column

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Quality control of LPG (Liquefied petroleum gas) produced in Debutanizer columns are essential for efficiency and profitability of Natural Gas Processing Units. In practice, however, the monitoring of quality parameters such as composition along the day is usually limited by the low frequency of laboratory testing, reliability problems of instrumentation and high maintenance costs. Implementation of advanced process control techniques for optimization and quality control of these products also demand an alternative online monitoring of these variables. Virtual sensors are mathematical models based on artificial neural networks that provide online measurement of variables based on current and historical values of other related variables. In standard applications, the use of artificial neural networks for virtual sensors are based on manual data pre-processing, offline training of a Multi-Layer Perceptron neural network and implementation using adjustable bias. This traditional way of implementation is difficult to maintain and prone to degradation of the network over time.

In this paper, a self-adjusting strategy to infer the composition of Ethane and LPG at the top of the Debutanizer Column will be presented. This work shows how the problems in relation to degradation and detuning facing new conditions of the plant were automatically adapted using Extreme Learning Machines approach.

This new methodology offers an alternative to what is routinely applied in the internal works of Petrobras, providing a robust, optimized, reliable and easy to use for the implementation and maintenance of virtual sensors, providing reliable data to operators and a solid foundation for implementation of an advanced process control (APC) strategies.

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Performance benchmarking and process development for converting CO2 into useful chemicals

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The current drive to prevent anthropogenic climate change by reducing CO2 emissions by capture presents a new challenge for its safe disposal or utilization. The easiest approach is to sequestrate the captured CO2. One of the relatively established processes is to use the captured CO2 for enhanced oil recovery through gas injection technique in depleting oil reservoirs. After the feasible recovery of oil, CO2 can further be injected into the reservoir until its saturation for storage. Although this is an effective technique, it only mitigates the problem for a short term. This is because such an approach is bound by the remote availability and limited capacity of such oil reservoirs. Thus, it is necessary to develop alternative and more sustainable approaches for CO2 reduction.

Among the available alternatives, a promising approach is to re-use CO2 in the chemical production chain as a renewable feed stock [1]. A number of reports and articles suggest the use of CO2 as a feed stock [1,2] for a variety of products such as urea, hydrocarbons, and polycarbonates. Of these, converting CO2 to fuels is of important consideration as it has a significant potential to reduce emissions. Methanol (MeOH) is one such important product, which can be directly produced from CO2 and is an important intermediate to useful products such as di-methyl ether (DME). Several researchers [3] have studied the production of methanol from CO2. Most of these studies focused on developing and identifying efficient catalysts for best reaction conversion. Kim et al. [4] studied a process for methanol production from CO2 using solar energy. Thus, only limited studies exist in the literature that either (1) benchmarks a CO2 reduction process or (2) analyse different process alternatives and their relative advantages.

In this work, we focus on two objectives: (1) benchmarking the energy and process efficiency of a CO2 to chemicals conversion process and (2) develop an efficient process model for the production of MeOH or DME from CO2. For this, we investigate a number of potential routes for synthesizing valuable products such as MeOH and DME from the conversion of CO2. We study the energy and process efficiencies of such identified process alternatives. In addition, to assess the relative performance of a given CO2 reduction process, we present a set of important performance indicators and establish benchmark values for such parameters from relatively mature industrial technologies. These performance indicators have the potential to serve as important metrics to measure the relative performance of new approaches.

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