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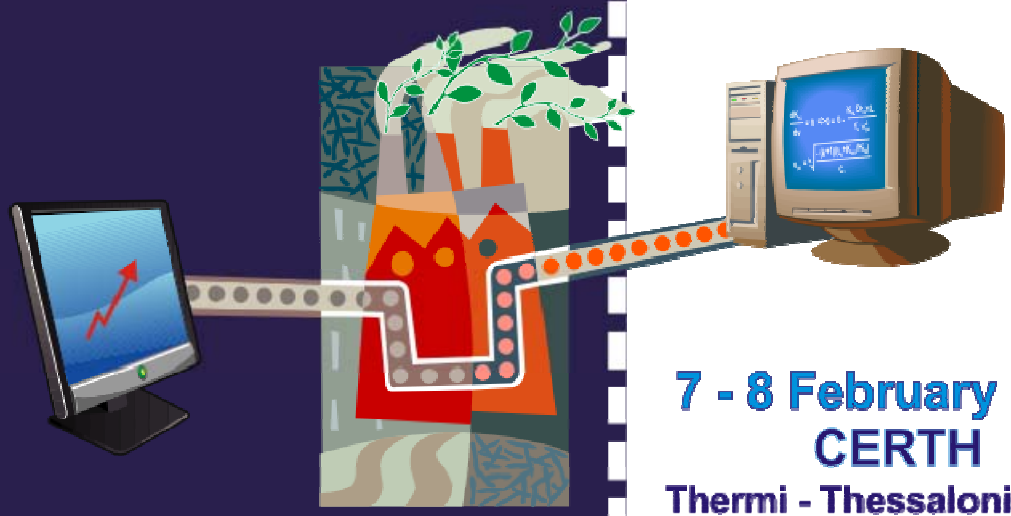

7 - 8 February 2008
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CAPE FORUM 2008

7-8 February 2008
CERTH Convention Hall
Thessaloniki, Greece

Thursday February 7th, 2008

08:30-09:15		***Registration***
09:15-09:40		Opening - Welcome
		Oral presentations S1 – Chairs: N. Vaklieva and S. Bezergianni
09:40-10:20	OP1.0	*Capturing Dynamics in Supply Chain Integrated Management* **L. Puigjaner** Universitat Politecnica de Catalunya, Spain
10:20-10:40	OP1.1	*"SC-MOPP" – Platform for Planning and Scheduling Multi-site Manufacturing Systems* **B. Ivanov**, J. M. Lainez, N. Vaklieva-Bancheva, K, Minchev, E. Shopova, L. Puigjaner, and A. Espuna Bulgarian Academy of Sciences, Bulgaria
10:40-11:00	OP1.2	*A Toolbox for Early Market Introduction of New Energy Technologies* **I. Bulatov** and J. Koppejan The University of Manchester, U.K.
11:00-11:10		***Coffee Break***
11:10-11:30	OP1.3	*Modelling the Intra-Particle Transport Phenomena and Chemical Reactions of Olive Kernel Fast Pyrolysis* T. Damartzis and **A. Zabaniotou** Aristotle University, Greece
11:30-11:50	OP1.4	*Improving the Maximum Conversion of Ethanol Esterification* **M. Emtir**, I. M. Mujtaba, and E. A. Edreder Libyan Institute of Petroleum, Libya
11:50-12:10	OP1.5	*Biorefinery: Analysis of Process Design Alternatives* **N. Al Haque** and R. Gani Technical University of Denmark
12:10-12:30	OP1.6	*Modeling and Simulation of Crystallization Processes for the Purification of Phosphorous Acid* **U. Brinkmann** and E. Kenig Universitaet Dortmund, Germany
12:30-14:00		***Lunch***
		Oral presentations S2 – Chairs: C. Botar and C. Chatzidoukas
14:00-14:40	OP2.0	*Process Performance Monitoring – Towards Model Based Approaches* **J. Morris** Newcastle University, U.K.
14:40-15:00	OP2.1	*A Systematic Approach to Optimization-Based Control of Wastewater Treatment Plants* **J. Busch** and W. Marquardt RWTH Aachen, Germany
15:00-15:20	OP2.2	*Multivariable Fuzzy-Neural Model of Polymer Process* **V. Chitanov** and M. Petrov Technical University of Sofia, Bulgaria
15:20-15:40	OP2.3	*Model Predictive Control of a Cyclic Propylene Steaming Pilot Plant* I. Anastasiou, C. Ziogou, K. Kostaras,S. A. Papadopoulou, **S. Voutetakis**, and P. Seferlis CPERI/CERTH, Greece
15:40-16:00	OP2.4	*An Adaptive Backstepping Technique for the Control of a Neutralization Process* E. H. El Mazoudi and **B. Messnaoui** Ecole Mohammadia d'Ingénieurs, Morocco

16:00-16:20	OP2.5	*Life Cycle Assessment Coupled with Process Simulation Under Uncertainty for Reduced Environmental Impact: Application to Phosphoric Acid Production* **A. D. Bojarski**, G. Guillin-Gosalbez, and L. Jimenez Universitat Politecnica de Catalunya, Spain
16:20-16:30		***Coffee Break***
16:30-18:00		Poster presentations SP – Chairs: P. Seferlis, S. Voutetakis
	PP01	*Model-Based Investigation of the Microbial Production of Polyhydroxyalcanoates (Phas)* G. Penloglou, A. I. Roussos, **C. Chatzidoukas**, and C. Kiparissides Aristotle University and CPERI/CERTH, Greece
	PP02	*Analysis and a Metabolic Interpretation of the Ph Evolution During Grape Must Alcoholic Fermentation* H. Akin, I. Touche, C. Brandam, P. Strehaiano, and **X. M. Meyer** ENSIACET, France
	PP03	*Energy Saving Potential of Phosphoric Acid Production by Wet Process* L. L. Tovazhnyansky, P. Kapustenko, L. M. Ulyev, and **S. A. Boldyryev** SODRU, Ukraine
	PP04	*Dynamic Simulation and Control Studies of the Main Fractionation Column of a Heat Integrated Fluid Catalytic Cracking Plant* **E. Jara-Morante**, R. Roman, and P. S. Agachi Babes-Bolyai University, Romania
	PP05	*Study of a Complex Petrochemical Process Based on Dynamical Mathematical Modeling Analysis* **R. Roman**, Z. K. Nagy, M. V. Cristea, E. Jara Morante, and S. P. Agachi Babes-Bolyai University, Romania
	PP06	*Application of Principal Component Analysis on a Hydrotreating Process* S. Bezergianni and **A. Kalogianni** CPERI/CERTH, Greece
	PP07	*The Simulation of Closed-loop Barometric Condenser System in Wet Phosphoric Acid Production Process* P. Kapustenko, **G. Khavin** and A. Perevertaylenko SODRU, Ukraine
	PP08	*A Non-Linear MPC Strategy for Feed Conversion Targeting in a FCC Pilot Plant* **I. Anastasiou**, S. A. Papadopoulou, S. S. Voutetakis, and P. Seferlis CPERI/CERTH, Greece
	PP09	*The Impact of Product Lifecycle on Capacity Planning Best Policies of the Reverse Supply Chain with Remanufacturing* **E. Athanasiou** Aristotle University
	PP10	*Generic Modelling, Design and Optimization of Industrial Phosphoric Acid Production Processes* **A. I. Papadopoulos** and P. Seferlis CPERI/CERTH, Greece
	PP11	*Operating Policy and Simulation Studies of a Stand-Alone Power System Using Renewable Energy Sources and Hydrogen Storage* D. Ipsakis, S. Voutetakis, P. Seferlis, **F. Stergiopoulos**, S. Papadopoulou, and C. Elmasides CPERI/CERTH, Greece
	PP12	*Oil Production Optimization in Petroleum Reservoir* **F. Razavi** and F. Jalali Farahani University of Tehran, Iran
20:30-24:00		***Conference Dinner***

CAPE FORUM 2008

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Friday February 8th, 2008

09:00-11:20		Oral presentations S3A – Chairs: L. Simon and P. Swinkels
09:00-09:40	OP3.0	*Microbial and Biocatalytic Production of Advanced Functional Polymers* **C. Kiparissides** and C. Chatzidoukas Aristotle University and CPERI/CERTH, Greece
09:40-10:00	OP3.1	*A Tool for Interactive Scheduling in Biopharmaceutical Engineering* **A. Koulouris**, C. Siletti, and D. Petrides Intelligen Inc., U.S.A.
10:20-10:40	OP3.2	*Global Sensitivity Analysis Techniques for Application on Dynamical Models of Biological Systems* **A. Kiparissides**, S. Kucherenko, E. Pistikopoulos, and A. Mantalaris Imperial College London, U.K.
10:20-10:40	OP3.3	*Recent Development and Novel Graphical Methods for CAPE* **H.–L. Lam**, F. Friedler, P. Varbanov, and J. Klemes University of Pannonia, Hungary
10:40-11:00	OP3.4	*Knowledge Domain Visualization in a Specific Field of Research. Case Study of Forced Unsteady State Reactors* **C. C. Botar-Jid**, A. Kraslawski, and P. S. Agachi Babes-Bolyai University, Romania
11:00-11:20	OP3.5	*Pollutant Transport Characterisation as a Function of River Characteristics and Pollutant Release Type* **C. Ani** and A. Kraslawski Lappeenranta University of Technology
11:20-11:30		***Coffee break***
11:30-12:30		Oral presentations S3B – Chairs: I. Bulatov and D. Missirlis
11:30-11:50	OP3.6	*A Grid Computing Prototype for Integrated Solvent and Process Design* **A. I. Papadopoulos** and P. Linke CPERI/CERTH, Greece
11:50-12:10	OP3.7	*A Systematic Methodology for the Selection of Green and Non-Reactive Solvents for Multistage Organic Reactions* **M. S. Bashir** and R. Gani Technical University of Denmark
12:10-12:30	OP3.8	*MINLP Synthesis of Reactive Distillation Column with MIPSYN* **M. Ropotar**, A. Totain, Z. Novak Pintaric, J.–M. Reneaume, and Z. Kravanja University of Maribor, Slovenia
12:30-12:50	OP3.9	*Study of an Integrated System for the Production of Hydrogen by Autothermal Reforming of Methanol* **D. Ipsakis**, M. Ouzounidou, P. Seferlis, S. Voutetakis, and S. Papadopoulou Aristotle University and CPERI/CERTH, Greece
12:50-14:00		***Lunch***
14:00-16:00		Oral presentations S4 – Chairs: R. Roman and A. Papadopoulos
14:00-14:40	OP4.0	*Meeting the Sustainable Freshwater Demand of Tomorrow's World by Desalination: State of the Art and Future Challenges for the CAPE Community* **I. Mujtaba** University of Bradford, U.K.
14:40-15:00	OP4.1	*Operation and Selection of Large-Scale Batch Distillation Equipments Considering Liquid Swelling* **L. L. Simon**, H. Kencse, and K. Hungerboehler ETH Zurich, Switzerland

15:00-15:20	OP4.2	*Optimization of a Gas Sweetening Unit* **B. Sohbi** and M. Meakaff Libyan Institute of Petroleum, Libya
15:20-15:40	OP4.3	*Experimental Characterization and CFD Simulation of Pressure Drop and Liquid Hold-up in A Structured packed Column* **M. Haghshenas Fard** Islamic Azad University, Iran
15:40-16:00	OP4.4	*Computational Fluid Dynamics Study on the Decomposition of Ammonia in a Selective Porous Membrane* **A. Sideridis**, D. Koutsonikolas, D. Missirlis, S. Topis, S. Kaldis, G. Skodras, and G. Sakellaropoulos Aristotle University, Greece
16:00-16:20	OP4.5	*Development of Advanced Polymerization Process Modeling, Simulation, Design and Optimization Tools Based on Interoperability Specifications* **A. Krallis**, V. Kanellopoulos, C. Chatzidoukas, P. Pladis, and C. Kiparissides Aristotle University and CPERI/CERTH, Greece
16:20-16:45		Closing remarks\

CAPE FORUM 2008 is organized under the auspices of ***Chemical Process Engineering Research Institute*** of the ***Centre for Research and Technology – Hellas*** and the ***Department of Mechanical Engineering*** of the ***Aristotle University of Thessaloniki***.

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Capturing Dynamics in Supply Chain Integrated Management

Luis Puigjaner

Universitat Politecnica de Catalunya, Spain

There is a large body of work on supply chain (SC) optimization in the chemical process industry (CPI). However, some of the basic aspects of the optimization problem are not adequately handled by the models and solution strategies developed so far in the literature. This presentation focuses on the underlying philosophy of our approach to supply chain management (SCM) in the CPI, which aims to overcome the challenges posed by this problem. Two main topics that offer great opportunities for improvement in SCM are discussed. These are the development of modeling approaches and solution strategies that reflect SC dynamics, the inclusion of environmental considerations, and the incorporation of novel business aspects and key performance indicators (KPI) into the existing formulations to enlarge the scope of SC analysis, which is currently rather limited. Our integrated solution strategy for SCM, which covers the aforementioned aspects and implements the ideas and concepts developed in our research, is also presented and its advantages are highlighted in case studies. Finally, a demonstration shows the dynamic interaction between different levels of the SC including local scheduling and rescheduling decisions, monitoring, diagnosis and control.

Back to program

"SC-MOPP" – Platform for Planning and Scheduling Multi-site Manufacturing Systems

B. Ivanov, J. M. Lainez, N. Vaklieva-Bancheva, K. Minchev, E. Shopova, L. Puigjaner, A. Espuna

Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria

Good planning is the base for better management of the multipurpose chemical complexes. It has to provide answers: which products, how much, when and where must be manufactured in the comprised plants during some horizon of interest. To do this, large amount of information concerning type of products, plants' capacities, market demands, possible suppliers of raw materials, type of transportation and respective costs must be taken into account. Moreover, planning of multipurpose chemical complexes is a hierarchy and iterative process. In it, at the top level, using Supply chain (SC) models, an optimal product portfolio for the entire complex and its distribution over the comprised plants are determined, while at the second level the best internal order, i.e. schedules, for products manufacturing in each plant has to be found. If needed, scheduling results turn back to the top level and use to improve plans on the next iteration. Assembled software package "SC-MOPP" goals to solve both, planning and scheduling levels for multipurpose chemical complexes. Determination of optimal product portfolio is carried out by the "SC" package. In it, five echelon supply chain model, comprising raw materials suppliers, plants, warehouses, distributors and markets is used. Using "SC" package, the supply chain structure, product portfolio and its distribution over the plants and support by the other SC elements can be determined so as to ensure maximal profit for the entire manufacturing complex. Solution of scheduling problem for each plant is provided by the "MOPP" package. Created schedules belong to the "job-shop schedules". The evaluation criterion is minimization of makespan. Both packages are integrated. Replica of the "MOPP" interface for data introducing is built in the "SC" package. Thus, main data required to solve scheduling problem are available at the first level. They are completed with product demands for each plant which are an output of the "SC" package. Using the XML language format forward and back communication between packages is ensured. Later provides opportunity for the iterative problem solution. The "SC" interface is oriented to the end user. The "SC" package is developed in the Institute of Chemical Engineering (Bulgarian Academy of Sciences). It is coded in MATLAB R2006a and is designed to work in WINDOWS-2000 environment. The "MOPP" is designed in the Catalan Polytechnic University. It uses as entrance the data provided by "SC" carrying the information about the multipurpose plants and calculated production demands. The package is coded in C++ and works in WINDOWS-2000 environment. Assembled "SC-MOPP" platform has an open structure and provides opportunity to be extended with new models and calculation methods.

Back to program

A Toolbox for Early Market Introduction of New Energy Technologies

Igor Bulatov, Jaap Koppejan

The University of Manchester, U.K.

The lead-time for the development of a new energy technology, from the initial idea to the commercial application, can take many years. The reduction of this lead-time has been the main objective of the EC DGTREN, who have funded two related recent projects, EMINENT and EMINENT2 (Early Market Introduction of New Energy Technologies) These projects were implemented in order to identify and accelerate the introduction and implementation of leading edge European technology in the field of energy saving into the market place. The principal features of the projects included the development of a software tool and an integrated database of new technologies and sectoral energy supplies and demands. The software tool has the capability to analyse the potential impact of new and underdeveloped energy technologies in different sectors emerging from different countries. In addition, the software tool has been used to perform Case studies which have been used to illustrate the new technologies.

Back to program

Modelling the intra-particle transport phenomena and chemical reactions of olive kernel fast pyrolysis

Th. Damartzis and A. Zabaniotou

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Abstract. In the present study the development of a mathematical model for the description of the pyrolysis of a single solid olive kernel particle and the prediction of the fast pyrolysis product yields, is presented. Kinetic model is coupled with heat transfer model. The global degradation of biomass is based on Koufopanos et al. mechanism and described by two parallel 1-order reactions. The analysis is focused on primary degradation for small particle and simulations have been carried out for a spherical particle, with radius of 175 μm. The model has been validated against experiments carried out in a laboratory wire mesh reactor, for temperature range from 573 K to 873 K and a heating rate of 200 K/sec. The results of the simulation are in good agreement with the experimental data, regarding temperature, conversion histories and product distribution of olive kernel fast pyrolysis. The numerical method applied was finite difference for the heat transfer model and Runge - Kutta 4^{th} order method for chemical kinetics model equations.

Keywords: Modelling; fast pyrolysis; kinetics; heat transfer; olive kernel; wire mesh reactor.

Back to program

Improving the Maximum Conversion of Ethanol Esterification

M.M. Emtir, I.M. Mujtaba and E.A. Edreder

Libyan Institute of Petroleum, Libya

In this study, the (catalysed) esterification process of acetic acid with ethanol producing ethyl acetate and water is modelled using detailed mass and energy balances and thermodynamic properties within gPROMS modelling software (version 3.0.3) [1].The basic model was taken from Mujtaba [2] assuming no azeotrope formation in the system. Kinetic and vapor-liquid equilibrium models from Bogacki et al. [3] and Suzuki et al. [4] respectively. The performance of batch reactive distillation is evaluated in terms of maximum conversion of ethanol to ethyl acetate. Five cases with varying amount of reactants (including the cases with the reduced amount of water in the feed and keep the amount of acetic acid and ethanol fixed) are utilised to improve the conversion of ethanol to ethyl acetate. The feeds <Acetic Acid, Ethanol, Ethyl Acetate, Water> are: Base Case - <2.25, 2.25, 0.0, 0.50>, Case 1 - <2.5, 2.5, 0.0, 0.0> Case 2 -<2.0, 2.0, 0.0, 0.0>, Case3-<2.0, 2.0, 0.0, 0.2> and Case4 -<2.0, 2.0, 0.0, 0.4>. The Optimization problem with varying batch time (between 5 to 25 hrs) is formulated to maximise the conversion while optimising the reflux ratio subject to product purity (0.7 mole fraction of ethyl acetate) in the distillate product. Piecewise constant and linear reflux ratio profiles (one interval) are considered as a control variable for the base case while only one constant reflux ratio strategy is considered for the other cases. The optimization results indicate that piecewise linear reflux ratio strategy is better than constant reflux ratio profile as a control variable to improve the maximum conversion of ethanol to ethyl acetate. Moreover, distillate product achieved when the column operated using optimal linear reflux ratio profile is higher than that using constant reflux ratio strategy. The effect of changing water amount in the feed, a comparison results between Case 1 and Base Case (The column operated at maximum capacity of the reboiler) shows that the conversion and the amount of product improve by about 3 % and 40 % respectively. The column can be also operated at lower reflux ratio profile compared with the base case. The optimal results in the cases (2,3 and 4) represented show that increasing of the water amount in feed leads to reduction in maximum conversion and the column is operated at higher reflux ratio compared to Case 2. Moreover, the distillate product decreases when the amount of water in the feed increased, which is proving that the reaction goes backward leading to reduction in conversion.

Back to program

Biorefinery: Analysis of process design alternatives

Naweed Al Haque and Rafiqul Gani

CAPEC, Department of Chemical Engineering, Technical University of Denmark.

The modern society depends on the chemical industries to supply chemicals for products used in homes, clothing, food, healthcare, water, transportation and many other items that are a part of daily life. These industries rely on the carbon in natural gas and petroleum to provide the basic building blocks or feedstock to produce the other items. The limited resources available from fossil fuels, coupled with environmental problems, have led countries to seek a new sustainable alternative. In the last few years, enormous progresses have been made in bio related engineering. This thesis deals with the concept of "White Biotechnology", i.e. the production of chemicals by either fermentation or enzymatic conversion.

Biorefineries represent complex (to fully integrated) systems of sustainable, environmentally and resource-friendly technologies for the comprehensive (holistic) material and energetic utilization. In addition to this, it allows us to use this process in the exploitation of biological raw materials in the form of green and residue biomass from targeted sustainable regional land utilization.

This study investigates the current opportunities of biotechnological production of chemicals. The objective is to be able to present a detailed investigation of techno-economic viability of white biotechnology to develop a biorefinery. Key research questions are: which products could be made with white biotechnology, whether these products contribute to savings of energy use and green house gas emissions, and under what conditions the products will become economically viable. The final result would be to create an integrated biorefinery network that will be able to produce a lot of tailor made chemical products.

Candidate chemicals were selected from a list of the top 50 chemicals determined by US DOE for building block materials. Chemicals such as lactic acid, 1, 3-Propanediol, Succinic acid and Ethanol are now being commercially produced at bulk rate. It has been decided upon to select these four chemicals because they have the possibility to compete directly against existing products derived from petroleum. There is a market already present for these chemicals, thus making it less tedious to evaluate the cost structures and growth potential of these chemicals.

Techno-economic analyses were performed for these chemicals using corn as the available biomass. It clearly illustrated that the products had a rising demand trend and it could be produced at cost competitive prices. Further economic analysis depicted a reasonable rate of interest and payback period could be attained. Optimization of profit has been performed on the biorefinery network using glucose feed rate as a variable. Targets for process improvements to achieve a more sustainable biorefinery network have also been investigated.

Back to program

Modeling and simulation of crystallization processes for the purification of phosphorous acid

U. Brinkmann and E. Y. Kenig

Technische Universitaet Dortmund, Germany

Crystallization from solution is widely used as a final purification and product formulation step for fine chemicals and pharmaceuticals as well as a unit operation for the separation of bulk chemicals, e.g. inorganic salts. In general, crystallization occurs in supersaturated solutions; the kinetics of crystal nucleation and growth is controlled by the degree of supersaturation. At industrial scale, supersaturation is reached by solvent removal (e.g. by evaporation) or by cooling of the solution. The selection of the appropriate process is usually based on the way the phase equilibrium depends on the temperature. Integration of both solvent removal and cooling can be realized either within one single stage or in a sequence of several units. Such integration helps to reach high purities and yields of the desired product. Model-based simulations represent a useful means to compare and optimize process variants. In this work, a process model for the description of cooling and evaporative crystallization in a batch operation mode is presented. Crystallizer description is based on the ideal stirred tank concept. In case of evaporative crystallization processes, the crystallizer is equipped with heating and with vapor outlet; in case of cooling crystallization, it is supplied with cooling facilities. The model comprises mass, heat and crystal population balance equations (see Brinkmann et al., 2008). The latter describe the distribution of crystal sizes in the suspension. It is assumed that the population balance depends only on the kinetics of crystal birth and crystal growth. It represents a nonlinear partial differential equation; to solve this equation, a solution method based on the moments of distribution is selected. In this approach, the population balance equation is reduced to a set of linear differential equations. The latter are discretized and solved numerically with the help of a Fortran-based code. To validate the model, the purification of phosphorous acid is simulated and the results are compared to experimental data of Butenko et al. (1997). In the experiments, the initial aqueous solution contained nearly equal amounts of phosphorous acid and sodium oxalate. After crystallization of sodium oxalate by solvent evaporation and cooling, approximately 5 wt % of its initial amount remained in solution. The simulated acid purities agree well with the experimental values for both crystallization stages. With the validated model, simulation studies are performed to develop an industrial-scale process for the purification of phosphorous acid. It is shown, that a combination of two stages (first evaporation, then cooling) is required to reach purities of phosphorous acid in the remaining solution higher than 90 wt %. Further, simulations are accomplished to investigate the influence of the cooling rate at the cooling crystallization stage. Among others, it was found that higher cooling rates result in smaller mean crystal sizes.

References:
Brinkmann, U.; Er, M.A.; Kenig, E.Y.; Butenko, Yu.V.; Koltsova, E.M.: Model-based design of a phosphorous acid purification process, accepted at 17th International Symposium on Industrial Crystallization, 2008, Maastricht.
Butenko, Yu.V.; Koltsova, E.M.; Vasilyeva, L.V.: Studying and modeling production of phosphorous acid from sodium phosphite solution. Russian Journal of Applied Chemistry 70 (1997), 1847-1850.

Back to program

Process Performance Monitoring – Towards Model Based Approaches

Julian Morris

Newcastle University, U.K.

In today's process manufacturing environment, a number of issues arise which can challenge the application of standard MSPC based process performance monitoring. Most methodologies are based on static PCA or PLS approach with only a few addressing the impact of process dynamics and auto-correlated data. The impact that process dynamics can have on the assured detection, diagnosis and sensitivity of the performance monitoring charts is becoming important. Earlier work has been provided by, for example Negiz & Cinar, 1997, Russell et al, 2000, Simoglou et al, 2002, McPherson et al, 2002, and Fletcher et al, 2002. This paper presents the use of Canonical Variate Analysis (CVA) and Autoregressive (AR) time series models for multivariate statistical process control based process performance monitoring systems which are discussed alongside two process simulation studies. One is based on a benchmark semi-batch styrene-butadiene rubber (SBR) emulsion polymerization (Nomikos and MacGregor, 1994) and the other on a free radical batch polymerization of methyl methacrylate (MMA), (Kiparissides et al, 2002). The dynamic approaches are compared with the standard multiway PCA (MPCA) batch unfolding approaches of Wold et al (1998) and Nomikos and MacGregor, (1994), and Dynamic and Adaptive PCA approaches. Three batch faults are considered, a reactor fouling problem, a reaction impurity problem and a control valve failure. Normal probability and autocorrelation plots of the residuals allow any non-normal and serial correlation to be identified in the removal of unwanted structure in the residuals to allow for appropriate statistical monitoring (McPherson et al, 2002). For on-line monitoring, a number of different monitoring statistics are considered alongside variable contribution plots for each monitoring statistic for fault diagnosis. The studies indicated that the model-based monitoring method not only reduces the time to fault detection while keeping the false alarm constant but also detects small faults rapidly. The concept and potential of using a dynamic, CVA and AR time series, batch modelling approaches are demonstrated and hopefully open the way for more studies.

Whilst the process performance monitoring using CVA takes into account the process dynamics and correlation structure of the process data, the monitoring statistics may still exhibit serial correlation. Consequently, the traditional statistical basis for calculating the control limits may materialise in an excess of false alarms since the CVA model states and model residuals may exhibit non-negligible serial correlation. A new methodology is suggested which uses CVA to develop a state-space representation of the process and then utilises the Generic Dissimilarity Measure (GDM; Kano et al. 2000) to detect a change in the time series distribution of the CVA model states and residuals. The GDM quantitatively evaluates the difference between two groups of data. Simulation results demonstrate the superiority of the proposed methodology over the more traditional metrics of Hotelling's T2 and the Q-statistic for detecting subtle faults. This paper also proposes a weighted combined contribution index for fault identification. The basis of this study is a benchmark simulation of a continuous stirred tank reactor.

Back to program

A systematic approach to optimization-based control of wastewater treatment plants

Jan Busch and Wolfgang Marquardt

LPT, RWTH Aachen University, Germany

Biological wastewater treatment processes represent a global and large scale industry. Although widely employed their operation still poses significant difficulties. The unknown biomass composition and degradation kinetics, the limited measurements information, and the highly dynamic inflow rate and inflow concentrations result in considerable uncertainty. Thus only simple control approaches are employed today. Critical component concentrations are typically kept within federal limits using single variable control loops. However, these simple concepts frequently lead to costly constraint violations and do not guarantee economically optimal operation.
In this talk we present the systematic development of a model-based control framework for wastewater treatment plants (WWTP). It focuses on the stepwise development and design of the hierarchical controller. The control framework is based on the concept of time scale separation: the disturbance and process dynamics are separated according to their time constants and assigned to different control layers. A dynamic predictive scheduling (DPS) layer responds to the slowest dynamics. It decides on the optimal sequence of operational strategies, which comprise the operational objectives and constraints and computes optimal setpoint trajectories for the states and the inputs. If these trajectories were implemented at the plant without further to do, suboptimal or even infeasible plant operation would result due to process disturbances and plant/model mismatch. Hence a non-linear model-predictive control (NMPC) layer is employed to force the process to track the setpoint trajectorie s. PID type base layer control realizes the updated inputs from the NMPC layer and rejects disturbances with fast dynamics.
Control models are employed by the DPS and the NMPC layer for the prediction of process behavior. These models require initial state estimates as well as estimates of uncertain model parameters. Hence a state and parameter estimation layer utilizes measurements from the process as well as process models to compute these estimates. The sensor network can be designed systematically to obtain an observable system at minimum cost. Finally the uncertain inflow rate and inflow concentrations need to be predicted.
Up to now model-based control approaches have not been implemented at real WWTP. Thus a sophisticated plant substitution model needs to be employed to test the proposed approaches in simulation scenarios.
Suitable models and algorithms need to be chosen for each of the control layers. The communication between the layers needs to be well-defined. Solutions are proposed for each of these questions. The modular design of the control framework is highlighted – it allows for the individual replacement or the restriction to a subset of the layers. The software implementation of the controller is discussed. It is shown how the use of the commonly available OPC interface allows the straightforward replacement of the plant substitution model by a real plant.

Simulation results are shown and discussed to undermine the proposed economical benefit of advanced model-based control approaches for WWTP and to demonstrate how the large amount of uncertainty in their operation can systematically be tackled.

Back to program

Multivariable Fuzzy-Neural Model of Polymer Process

V. Chitanov and M. Petrov

Technical University of Plovdiv, Bulagaria

The obtaining an accurate and comprehensive multivariable mathematical model of the polymerization process is of strategic importance to the control engineering purposes in the polymerization industry. It is characteristic for these processes a grate non-linearity and many difficulties applying traditional estimation techniques. This paper describes an approach based upon multivariable neural-fuzzy representation of the model. A concrete model is constructed with the Sugeno fuzzy inference technique by applying state space implementation in the local rules for modelling the dynamic behavior of the polymer process. Such multivariable neural-fuzzy models of polymer quality could be used successfully for optimization and control of polymerization processes. A short example for such implementation is included with additional results for modeling of the main characteristic parameters of the polymer process.

Back to program

Model Predictive Control of a Cyclic Propylene Steaming Pilot Plant

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The industrial production of catalysts is very demanding as far as the quality of its products is concerned. Due to that reason their proper evaluation is considered to be a necessity. The Cyclic Propylene Steaming Pilot Plant (CPS) is a fluidized bed reactor established at Chemical Process Engineering Research Institute (CPERI) which is used for catalyst deactivation. In order to ensure the creditability of the deactivation results one must have a reliable mathematical model that accurately simulates the systems behavior. The development of the mathematical model and the parameter estimation has been achieved and validated using open-loop dynamic experimental data and advanced statistical methods. Furthermore, the improvement of the overall control scheme has been achieved through a model-based predictive control strategy in order to have a more accurate control of the reactor's temperature, the energy requirements and the final product quality. The optimal sequence of the manipulated variables, which minimize the difference between the desirable and the predicted reactor temperature trajectories, is being calculated with dynamic programming techniques. The model predictive control strategy leads to superior performance in comparison to the previously installed system, consisted of conventional PID controllers.

Back to program

An adaptive backstepping technique for control of a neutralization process

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The control of pH is a very important problem in many processes, particularly in effluent wastewater treatment. The development and solution of mathematical models of these systems is, therefore, a vital part of chemical engineering dynamic modelling. A pH is difficult to control due to its nonlinear dynamics with uncertainties and its time varying properties. As the process to be controlled is highly nonlinear, the classic controller as PI and PID is not able to control these systems adequately. For this purpose, an adaptive pH controller is proposed to control the pH process. This nonlinear controller is designed using adaptive backstepping technique. A nonlinear optimization method is applied to fit the parameters of controller from experimental data related to pH vs. time. In the present study, in order to show the control performance and robustness of the proposed control strategy to the measurement noises and modelling errors, we consider the following pH process simulation: the first feed stream is composed of HCl + 0.02 mol/l H3PO4 and are replaced by the second feed composed of HCl+0.02 mol/l H3PO4 + 0.02 mol/l CH3COOH at 1500 s and at 2500 s, it is replaced by the third feed stream composed of HCl+0.02 CH3COOH mol/l.The reactor volume V = 5 litres, the feed flow rate Fin = 1 l/min, the maximum flow rate of the titrating stream Umax = 0.6 (l/min), the total ion concentration of the strong base in the effluent stream Cbo = 0.2 (l/min) and the total ion concentration of the strong base in the titrating stream Cb = 0.04 (l/min).

Based on the simulation results of the present study, the following general conclusions may be made: i) the proposed method shows a good control performance and robustness to the measurement noises and modelling errors; ii) we could recognize that the proposed control strategy shows robustness to the time constant of the pH sensor and the measurement noise; iii) the modelling errors in the feed flow rate and the reactor volume cannot almost affect the control performance and iv) the effect of the variation of the feed composition with modelling errors which consists on an uniform random number with a minimum equal zero and a maximum equal to 0.003.

Back to program

Life Cycle Assessment coupled with process simulation under uncertainty for reduced environmental impact: application to phosphoric acid production

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Environmental impact is measured through the CML 2 baseline 2000 V2.03, an environmental performance measure based on the concepts of Life Cycle Assessment (LCA). The task of generating reliable data for the LCA calculations is accomplished by using process simulation based on first principles models. Furthermore, uncertainty arising from industrial data and simulation hypothesis is explicitly incorporated by using Monte Carlo sampling, which allows translating statistical information into a set of representative scenarios for which the LCA calculations are performed. The combined use of LCA, process simulation and sampling techniques results in a powerful environmentally conscious quantitative tool that aims to guide decision-makers towards the adoption of more sustainable process alternatives. This novel methodology is applied to the specific case of phosphoric acid (PA) production.

Back to program

Microbial and Biocatalytic Production of Advanced Functional Polymers

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A premier initial interface between biotechnology and materials science is the utilization of biosynthesis and biocatalysis for the production of novel biomaterials with specified properties. Industrial biotechnology or "white biotechnology" is an emerging field that uses enhanced microorganisms like yeast, moulds, and bacteria as "cell factories", along with the enzymes derived from them, to produce high-added value specialty biopolymers from renewable sources. The present study aims at the development of novel sustainable biosynthetic and biocatalytic processes for the production of high-added value bioproducts (e.g., advanced functional lactic acid- and PHA-based polyesters with desired molecular properties, water-soluble chitosan and alginate biopolymers, functional polysaccharide-based biosurfactants), not accessible by conventional chemical technologies.

Synthetic polymers have been associated with a large variety of practical applications of every-day life with food applications as the most representative ones. However, the growing reliance on these polymers has raised a number of environmental and human health concerns. Most of these materials are neither biodegradable nor derived from renewable resources. In the last decades there has been an increasing interest towards the production of polymers from biological precursors by applying modern biotechnology. Certain biopolymers are very similar to conventional polymers (i.e., polypropylene and polyethylene) and, provided that their production becomes economically viable, could be considered as attractive alternative materials. However, with regard to polymer synthesis, successful examples like the production of polylactic acid from cornstarch are rare. Other processes like the microbial synthesis of poly-β-hydrobutyric acid still suffer from poor life-cycle analysis impact. Current research efforts are directed towards the production of high-added value specialty products, commodity polymers and the exploitation of specific advantages offered by the superior stereo- and regio-selectivity of the bioprocesses, for the biosynthesis of functional molecules.

Despite the advantages regarding sustainability and selectivity of product formation, biocatalysis is still not viewed as a first-line alternative, but only as a last resort when other synthetic schemes have failed. Major technological advances are needed to influence industry in adopting enzymic/microbial production routes. To address this challenge, the following radical innovations need to be pursued:

- Novel biocatalysts: Exploration of native or manipulated microorganisms for the low-cost production of a wide spectrum of tailored enzymes with respect to substrate specificity, reaction rate, thermal stability and optimum pH. Improvement of the stability, performance and catalytic efficiency of enzymic systems using immobilization technologies. Biocatalysis in organic media.
- Metabolic pathway engineering of multiple reactions to generate novel metabolic products, for enhancing naturally occurring pathways to generate intermediates and to broaden the utilizable substrate range to various renewable and waste carbon sources.
- Innovative downstream processing operation for the recovery of bioproducts.
- Digital bioproduction and bioprocessing: The application of advanced modeling, monitoring and control methods to the inherently complex and time varying nature of bioprocesses will bring new prospects for substantial improvements in production efficiency and product quality.

It is the objective of the present study to explore the microbial-based and novel biocatalytic routes for the production of specialty biopolymers based on a limited amount of bio-based platform chemicals derived from renewable sources.

Back to program

A tool for interactive scehduling in biopharmaceutical engineering

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Biomanufacturing possesses features that make scheduling unique. Primary equipment are more-or-less dedicated to specific processing steps, wait time between steps is usually zero, and changes to the main process are often avoided due to the heavily regulated nature of biomanufacturing. The inflexibility in the primary process means that any scheduling-related benefits should be sought in the ancillary operations where, however, most scheduling conflicts exist. It is a well-known fact in biomanufacturing that bottlenecks usually arise in the use of shared CIP (Clean-In-Place) and SIP(Steam-In-Place) skids for equipment and line cleaning or mobile tanks and transfer panels for material transfers. A scheduling tool that provides a very rich and very unique representation of the auxiliary operations and resources is presented. When it comes to scheduling, the key to resolving conflicts is to know where to add and exploit flexibility. Involving the user in the decision process ensures that the generated solutions are realistic and acceptable albeit not necessarily optimal.

Back to program

Global sensitivity analysis techniques for application on dynamical models of biological systems

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The ever increasing knowledge and understanding of biological systems necessitates the development and implementation of even more sophisticated and complex mathematical models. An inherent problem with the development of high fidelity models, especially ones representing complex biological systems, is the increase in the number of parameters. Furthermore, as current analytical techniques in cell biology do not allow the measurement of all parameters, experimental estimation of an extensive number of parameters often is an infeasible task (Sidoli et al. 2005).
Previous research in the field of mathematical modelling of biological systems has shown that statistical tools such as GSA can provide a guideline towards optimal experimental design, minimising cost and experimental labour (Kontoravdi et al. 2005, Rodriguez-Fernandez et al. 2007). GSA offers a comprehensive approach to model analysis (Saltelli 2000). Unlike local sensitivity analysis, GSA methods evaluate the effect of a factor while all other factors are varied simultaneously, thus accounting for interactions between variables without depending on the stipulation of a nominal point. Furthermore GSA allows the exploration of the space of possible alternative model assumptions and structure on the prediction of the model, thereby testing both the quality of the model and the robustness of the model based inference. The performance of GSA methods has, up to now, been tested on test functions with known analytical solutions and a limited number of parameters. Herein, we present for the first time an overview of the performance of GSA methods, deemed to be suitable for use in complex ODE or PDE models containing nonlinearities and coupled terms, such as biological or reaction network models. We examine a simple biological model consisting of 6 differential equations and 16 model parameters. A computational comparison between the established Sobol' indices and a novel method, namely derivative based global sensitivity measures is performed on the aforementioned model.

Back to program

Recent Development and Novel Graphical Methods for CAPE

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This is an overview of the recent development and application of graphical methods in process synthesis, which is one of the most challenging CAPE problems. The main goal of the process synthesis is the identification of the best process system or flowsheet structure that fits the requirements imposed to design. For a chemical process, this could be the conversion of raw materials into the final products, or the separation of a multi-component mixture. Several approaches have been used in solving the process synthesis problems namely the heuristic evolutionary and hierarchical decomposition approaches, as well as superstructure optimization. To support the synthesis, various graphical tools have been developed and intensively extended. They could simplify the problem by providing clear insight into problem major tradeoffs, which make it stand out among other methods especially when the CAPE is applied. The graphical methods are quick, flexible, and easy to use and make visual sense. This can be used for presentation, communication purposes and visualisation tools for non-expert decision-makers to whom the details of optimization models may be intractable. The intensively developed P-graph and established Pinch analysis are good examples of powerful graphical tools that demonstrated their adaptability in the process synthesis. P-graph is introduced for a structural representation in the process network synthesis, which simplifies the rigorous super-structure (maximal structure) by using a directed bipartite graph. P-graph has two types of vertices (one for operating units and another for the objects representing material or energy flows/quantities) which are connected by directed arcs. To obtain the optimal process solution structure, the maximal structure is broken down into the feasible structures, and followed by an optimisation analysis. Pinch analysis has been extensively used in chemical engineering for the minimization of the comsumption various resources such as energy and water. The original idea of pinch analysis is to graphically plotting ‘quality’ versus ‘quantity’. In the typical application for heat recovery systems the quality is temperature while the quantity is heat duty or enthalpy content. The heat demand and supply composite curves are clearly presented on the graph which gives users greater insight into the heat exchanger network synthesis problem. Both of these efficient graphical tools have been widely extended to several of disciplines and applications. The principles, development and the future applications of these two graphical methods are highlighted to demonstrate the implementation of the graphical methods and their potential development in CAPE. The proper synergy of P-graph and pinch analysis could be very beneficial for process synthesis particularly in CAPE applications.

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Back to program

Knowledge domain visualization in a specific field of research. Case study of forced unsteady state reactors.

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Starting a research in a new field requires tedious and hard work to find out, structure and gather the knowledge needed to deal with new problems. Identifying the most important aspects and changes in a specific knowledge domain represents a challenging task not only due to the complexity of a given research field but also because of the scale, diversity and/or domain dynamic nature. A key to solve the above mentioned problems is a use of methods for progressive knowledge domain visualization. The primary motivation for their use is a significant reduction of time for finding out and systematisation of information about a specific field of research. The visualisation methods apply techniques that may be used to identify temporal patterns associated with significant contributions, with their corresponding information, as a domain advances in time. In this way the latest developments in a specific research domain, the directions and new challenges for research and development, networking and contacts may be provided in a fast and easy way. In this approach, many aspects of a scientific field can be represented in the form of visually salient features which further may provide the way for knowledge identification. This work attempts to provide a methodology for knowledge identification in a specific field of research. Our approach, based on the use of CITESPACE software, facilitates structuring of knowledge, in the field of forced unsteady state reactors, which is needed when making design decisions.

Back to program

Pollutant transport characterisation as a function of river characteristics and pollutant release type

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It is very important to know the dependence of pollutants transport in the rivers as a function of hydrological and hydrodynamic characteristics (e.g. river channel width, river bed slope, water depth, water flow). This is required in order to ensure a sustainable development of the environment. To illustrate pollutants propagation a modelling of Somes River is studied, taking into account morphological, hydrologic and hydrodynamic characteristics. For each parameter of the model (e.g. river bed slope, river channel width, water depth, dispersion coefficient, water flow and velocity) specific dependence on the river length was determined taking into account the river channel particularities, and the fact that river parameters are also affected by the seasons of the year. For this task we used experimental data collected in 12 monitoring points along 421 km of river. At the same time different types of pollution (e.g. continuous, short time), different transport processes (e.g. diffusion, advection) and transformations taking place were considered in order to build the models. The purpose of this study is to show how river characteristics affect pollutants transport. The tools that we use are two predictive models for the cases of point and non point release. These models are used to illustrate dynamic distribution of pollutant concentration in river when the level of water changes, when the water flow increases because of rain, and also when other parameters modify. The simulation results show that river characteristics influence dispersion-convection dominance, affecting pollutants transport along the river, and changing river water quality.

Keywords: pollutants transport modelling, river hydrology, river hydrodynamics, Somes River characteristics

Back to program

A Grid Computing Prototype for Integrated Solvent and Process Design

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Grid technologies have received a lot of attention by the scientific community recently; however, developments are at their infancy and very few engineering applications have been reported to date. The Process Engineering domain makes an interesting application area for Grid technologies as the problem solving and decision-making generally involves multiple software and data resources and heavy computations. There are also numerous highly computationally demanding computer aided chemical engineering applications that can benefit from distributed Grid computing such as molecular simulations and large-scale optimisations. In theory, Grid technologies would enable distributed decision-support systems that could integrate all the required sources for process design activities, whether available in-house or from external sources, in a unified environment and make available vast computing power to tackle computationally intense problems. Such systems could significantly improve the design efficiency. We have set up a prototype Grid for integrated process and molecular design to demonstrate the potential of Grids in the Computer-Aided Process Engineering (CAPE) arena. The design problem makes an ideal candidate to investigate the potential of Grid technologies, to identify implementation difficulties and to highlight technology shortcomings. The prototype integrates a number of software resources (computer-aided molecular design (CAMD) tools, data mining tools for the analysis of molecular design information, process synthesis tools, web mining tools) and data repositories (in-house and web databases) required in the different design stages. The prototype also facilitates distributed Grid computing to tackle the computationally demanding process synthesis calculations. The user interface is a web portal designed under consideration of the design workflow and its possible variations. We will focus on the architecture of our prototype Grid and discuss its implementation together with the problems we faced and the lessons learned in the process. An application in integrated CAMD and process synthesis in liquid-liquid extraction will be presented.

Back to program

A Systematic Methodology for the Selection of Green and Non-Reactive Solvents for Multistage Organic Reactions.

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Solvents find indispensable use in pharmaceutical and fine chemical industries to facilitate the reaction-based separations by dissolving and/or bringing them together according to the specific operating conditions. Because of the excessive consumption millions of tons of solvent have to be disposed off every year putting a lot of emphasis to find the better green solvents that can replace the existing ones. In this study, we aim to use computer aided molecular design (CAMD) approach to select the solvents that, when used for multistage organic reactions will be benign for the reacting system and simultaneously minimize the environmental impact as well. For the information available and predicted about reaction mixture, the objective is to find the solvents that can promote the reactions and rank them according to the established scoring system. For the current study, the basis is the method developed by Gani et al , on the selection of solvents for the promotion of organic s ynthesis. This method incorporates the industrial practice knowledge about computer–aided design of solvents and property prediction. It involves multi-step algorithm primarily consisting of two stages. In the 1st stage, from the list of solvents that are commonly used in industry, candidates' fulfilling the pure component properties are scored according to a rule based algorithm. Simultaneously, CAMD technique is used to generate the candidates for the prescribed pure component property constraints and the generated candidates are then scored. In the second stage, the solvent candidates are further evaluated based on their mixture and reaction properties. This method now has been extended to handle more complex multistage organic reaction systems. In the final stage, a matrix of promising solvents is prepared in order to identify the solvents that can be used in more than one reaction stage. The ideal situation is that a single solvent can be used in all the reaction stages or a minimum number of solvents are used. The method is also extended to verify the reactivity of the identified solvent candidates with each compound of the reacting mixture. This involves the setting up of a stoichiometeric reaction (based on atomic balance) and then calculating the equilibrium constant (K) for the reaction, using pure component heat of formation data. The possible reactions routes are checked for each solvent-reactant or product reaction scheme and the calculated value of K determines if the solvent is inert or not. The presentation will highlight the solvent selection strategy through a case study from the pharmaceutical industry.

R Gani, C J Gonzalez, D J C Constable., Computers and Chemical Engineering, Vol. 29 1661-1676, 2005.

Back to program

MINLP synthesis of reactive distillation column with MIPSYN

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In order to develop optimization models for process industries, detailed process models are required, that provide accurate description of the process where several detailed calculations have to be included, like enthalpy, kinetic, equilibrium, efficiency and other equations. In our case such a complex model describes reactive distillation, which combines two processes in the same unit: chemical reaction of the reactants and the separation of products in a distillation unit. Reactive distillation has numerous advantages concerning the economic benefit and quality of the products, e.g. reduction of investment cost because several operations are united in one single process unit, utilization of reaction heat to reduce hot utility in the reboiler, improved selectivity of the reaction because of continuous removal of the products and thus, better quality of the products, and avoidance of the azeotropic mixtures. Such detailed models are large and complex and thus, difficult to solve. Therefore, the main objective of our work is to develop strategies for facilitating modelling and solution of such complex MINLP problems with an MINLP process synthesizer MIPSYN, the successor of PROSYN1. MIPSYN is a modular computer package for mixed-integer nonlinear synthesis of process flow-sheets, which enables automated simultaneous topology and parameter optimization of processes. It relies on the Modified Outer Approximation/Equality Relaxation MINLP algorithm and utilizes GAMS interface (General Algebraic Modelling System).
One of the main ideas of our research is to upgrade the MIPSYN package for implicit models using GAMS's external equations capabilities which is especially important when a part of a model is so complex that cannot be solved in equation-oriented environment. Although GAMS, as MIPSYN's interface, provides a powerful language for manipulating data and defining highly structured collections of variables and equations, there are situations when some parts of the model could be defined using FORTRAN, C++ or some other language user defined routine. This could be favourable because the size of the original optimization model is reduced if some extensive calculations are accomplished outside the optimization model, and several libraries of models already exist in FORTRAN, e.g. libraries of thermodynamic models, which can be easily connected into the optimization model. In previous work devoted to reactive distillation several applications for connecting GAMS models with FORTRAN routines have been developed. The attempts were successful for nonlinear programming (NLP) applying GAMS solver CONOPT, however, the convergence was not achieved by MINLP models applying DICOPT solver. Therefore, the objective of this and forthcoming research is to overcome the drawbacks observed by DICOPT solver and to upgrade the MIPSYN's MINLP algorithm for the use of external routines in combination with disjunctive programming and convex hull formulation of the problem. Better outcomes are expected with this algorithm especially because MIPSYN allows the user to interfere and assist the optimization subiterations during the main iterations of the optimization algorithm. For example, detailed initialization of each NLP subproblem can be performed before the execution of the NLP. This increases the chances for achieving the convergence of the MINLP reactive distillation problem described above.

Keywords: Reactive distillation, NLP, MINLP, MIPSYN

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Back to program

Study of an Integrated System for the Production of Hydrogen by Autothermal Reforming of Methanol

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All the developed as well as the developing world today is greatly concerned about the continuous problems of the environmental pollution as well as for the continuous increase on the price of oil. For this reason, the study and development of applications that deal with the production of alternative fuels and aim in the reduction of dependence from conventional fuels like oil and in the reduction of air pollutants acquire particular importance.
A methanol reforming fuel cell system, which consists of a methanol auto-thermal fuel reactor, a preferential oxidation reactor and a PEM fuel cell system has been designed and developed at C.P.E.R.I. (Laboratory of Environmental Fuels and Hydrocarbons). The main target of the project is the design of an autonomous integrated system with a capacity of 1-10 kW_e electric energy and also the development of a mathematical model that will be used for system evaluation.
The process of hydrogen production via autothermal reforming of methanol, consists of the methanol reformer and the preferential oxidation reactor for CO removal. Thus, the pilot plant in C.P.E.R.I. comprises the preheater, the autothermal reformer, the preferential oxidation reactor and a PEM fuel cell. The produced hydrogen along with other gaseous products (CO_2 and CO) is fed to the preferential oxidation reactor for the removal of CO at levels of 20-50 ppm, as it is well known that higher quantities of CO can poison the anodic electrode of the fuel cell and degrade its performance. The effluent stream of the preferential oxidation reactor consists of a gas mixture with a typical composition of 55-65% H_2, 15-25% CO_2, 15-20% N_2, 20-50 ppm CO in dry basis, which is introduced to the PEM fuel cell anode chamber. One of the most important advantages of this proposed method is that the process is taking place at lower temperatures compared with the reforming temperatures of other organic compounds like methane.
This integrated system has been studied from a theoretical and from an experimental scope at CPERI (Chemical Process Engineering Research Institute). The developed mathematical model consists of the energy and material balances that describe the behavior of the autothermal reformer and the preferential oxidation reactor. In the first steps of the theoretical analysis, the steady-state performance was studied where the various H_2O/CH_3OH ratios and various reaction temperatures revealed the same behavior as with the experimental study. The main variables that are concerned for the theoritical study are the concentrations of methanol, carbon monoxide, carbon dioxide and hydrogen as a function of the response time and the reactor length at both reactors. Moreover, the present work examines the effect of the inlet H_2O/CH_3OH and O_2/CH_3OH ratios and of the reforming temperature on methanol conversion and CO selectivity. From preliminary studies, it was found that higher temperatures led to higher H_2 concentrations but the CO level increased.

Furthermore the increase of the H_2O/CH_3OH ratio proved efficient as the CO reduced due to the water gas reaction and H_2 is slightely increased.
For future studies, the dynamic model will be developed in order to describe better the transient responses on the system. The evaluation of the mathematical model with experimental data will be another crucial step towards the development of a "plant wide" model based control. Dynamic simulations of the integrated system as a whole after studying each subunit separately, are used as the basis of developing end evaluating a ''plant wide'' model based control strategy. This strategy will exploit the inherent time scale separation in such integrated systems and involves the stabilization of individual subsystems in a fast time scale and supervisory control of the overall integrated system in a slow time scale.

Back to program

Meeting the Sustainable Freshwater Demand of Tomorrow's World by Desalination: State of the Art and Future Challenges for the CAPE Community

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Water is essential to all living species on earth and quality water must be available in abundance to all species. In addition, agriculture and industry require sustainable water supplies throughout the world. Global water shortages will become so catastrophic over the next decades that two in three people on the planet will face regular depletion of water supplies. Global thirst will turn millions into water refugees. Even Europe is showing warning signs. Agricultural land from Portugal to Greece is becoming more arid and some countries, notably Spain, are attempting to alleviate domestic shortages by buying water from abroad. Increase in population and standards of living together with water pollution are diminishing the quantity of naturally available fresh water while the demand for it is increasing continuously. Fresh water consumption is increasing at the rate of 4-8%/yr, 2.5-times the population growth. As more than 94 percent of the world's water is saline, desalination technology is vital for sustaining human habitation (including agriculture and industry) in many parts of today's world. The commonly used industrial desalination processes can be classified broadly into two groups: (a) Heat consuming or thermal processes (b) Power consuming or membrane processes; thermal process being the oldest and most dominating for large scale production of freshwater in today's world. While there is no shortage of research work in desalination for the last few decades, the ongoing objective has still been to improve the design, operation and control of desalination processes (mainly thermal) to ensure quality water at cheaper price with lower environmental impact. While membrane based processes are becoming cheaper with new development of membranes, thermal processes are still very energy intensive (energy being supplied by steam) and are cause for concern for environment. In addition, with seasonal seawater temperature variation the common industrial practice is to operate the thermal based plants at high temperature in summer. This leads to the use of increased amount of anti-scalant to reduce fouling and corrosion of heat exchangers (and plant equipment). Although this reduces frequent shut-down of the plant but causes further environmental problem associated with the added chemicals. Interestingly, most reported literatures on desalination are experimental based. There are only few published work dealing with rigorous mathematical modelling, mathematical optimisation and model based control. Computer Aided Process Engineering (CAPE) or Systems Engineering based research in tackling design, operation, optimisation, control, scheduling and maintenance are almost non-existent. This paper will highlight the state of the art and challenges for the CAPE or Systems Engineering Community to address sustainable freshwater demand of tomorrow's world by desalination technique.

Back to program

Operation and selection of large-scale batch distillation equipments considering liquid swelling

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In a multipurpose chemical batch plant many products are produced and separated using the same equipments; thus the design part is fixed and the process operation should be modified such that it is feasible to be carried out in the existing units. This situation brings up the challenge of the optimal equipment selection and pairing from a pool of existing equipments.
In multipurpose batch plants batch distillation is carried out using a standard size (Ciba-Geigy Technische Unterlagen) (2.5 m3, 4 m3, 6.3 m3) heated vessel (pot) which is connected to a rectification column with a certain number of trays and specified diameter. Since the process has to be performed in a non-dedicated setup, it can be easily recognized that depending on the operating parameters (temperature, pressure, pot filling degree, and substance physical properties) the maximum production rate can be limited by the distillation column flooding and the still pot liquid swelling. The reboiler content swelling occurs when the vessel content level rises due to the vapor stream that passes through the liquid caused by boiling. This phenomenon can produce significant productivity losses if it is not considered during process operation; improved process conditions during the operation of a batch reactor with respect to swelling have already been proposed in the form of an optimal control optimization (Simon et al., 2007). This work deals with the analysis of the industrial batch distillation operation, carried out in standardized equipment sizes, with regard to the main limiting factors: column flooding and the liquid level rise in the pot. While column flooding for distillation has already been studied during the last years, the liquid swelling in the pot has received less attention. Our work aims to identify these limitations for the most relevant standardized equipment sizes and to propose debottlenecking strategies. This contribution uses well established correlations in order to calculate the flooding and weeping (Stichlmair and Fair, 1998). In order to calculate the swelled liquid height in the reboiler vessel several hydrodynamic models are presented and compared: the bubbly model, Churn turbulent model (Fisher et al., 1992), Kataoka-Ishii model (Kataoka and Ishii, 1987). Finally, the Churn-turbulent hydrodynamic model is chosen and implemented. As a case study example a mixture of toluene and ethylbenzene is taken in order to be separated at 1 bar using a reboiler vessel size with nominal size of 6.3 m3 and a rectification column with a diameter of 0.5 m. The analysis results show that at 24 kmol/h vapor rate in the reboiler vessel swelling is caused, while this vapor rate in the rectification column is in the normal operating range. More simulations at low pressures (350 mbar) show that the liquid swelling in the pot limits the productivity even more severely; in order to increase the distillate production rate the pot charge (filling degree) should be lower thus the batch size as well. This situation rises new optimization opportunities in order to find the best compromise between a fast operation and a large batch size.

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Back to program

Optimization of a gas sweetening unit

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Units designed with selective amines often have little margin for error with respect to plant capacity. The equipment size, circulation rates, and amine concentration are very important for gas sweetening processes design. In this present paper, a simulation study has been investigated to optimize a gas sweetening unit using the software program (Hysys). The aim of the study is to investigate the effect of mixed amines as solvent, different circulation rates, different amine concentration, number of treys in absorber column, up on the gas treatment processes. The temperature profile increase with increase the number of trays and the absorbed amount of CO2 and H2S decrease with increase number of trays. The using of mixed amines can improve the gas treatment process. The temperature of rich amine decrease with increase the circulation rate in all different percent of mixed amines and different percent of MDEA without mixed. The water losses increase with increase the circulation rate in all different percent of mixed amines and different percent of MDEA.

Keywords— Simulation, Natural gas, alkanolamine process, gas sweetening processes.

Back to program

Experimental Characterization and CFD Simulation of Pressure Drop and Liquid Hold-up in A Structured packed Column

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Pressure drop and Liquid hold-up for two-phase flow in a structured packed column were simulated using a commercial CFD package, CFX version 10. Pressure drop experiments were measured with the Air / Water system. The experiments were carried out in a 0.073m diameter column, with an element of a ceramic structured packing (MELLADURE) of 0.053m in height. Pressure drops at the flooding and loading points are approximately 173 and 580 pa/m of packing, respectively. Pressure drops calculated from the CFD model were compared to its experimental counterpart. The average relative error between CFD predictions and experimental data for prediction of dry pressure drop and irrigated pressure drop are 20.3% and 23% respectively. In all cases, the CFD predictions show a good agreement with the experimental data.

Back to program

Computational fluid dynamics study on the decomposition of ammonia in a selective porous membrane

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The development of alternative technologies for the removal of gas pollutants at the integrated gasification combined cycle is considered as an important aspect for the environmental friendliness of energy production. During coal gasification, N2 contained in coal is converted to NH3. As much as 50% of the ammonia in the fuel gas can be converted to nitrogen oxides in the gas turbine when the gas is combusted to produce power. The temperatures encountered in these power generation systems are far above the temperature range for conventional chemical or physical absorption systems. Water based NH3 removal, for example, involves cooling the gas to about 120°C. To meet emission standards while maintaining the thermal efficiency of the process, the fuel gas should be cleaned at high temperature and pressure. At these conditions, decomposition seems to be the only solution for NH3 removal. The application of a high temperature catalytic membrane reactor process integrally linked with the gasification process appears to offer a unique route toward an efficient and cost effective method of removing the NH3 from coal gasification gas streams. This is because membrane based separation systems possess low energy consumption, reduced environmental impact, low costs of maintenance, space and weight efficiency and are relatively easy to install and operate. Chemical conversion and product purification take place in the same device. By the selective permeation of H2 through the membrane, it is possible to achieve significant enhancement of NH3 conversion. However due to the nature of the process the performing of precise experimental measurements at the direct vicinity of the selective membrane is relatively difficult and, thus, in order to investigate thoroughly the behaviour of such selective membranes, numerical methods can be used. Especially for axis-symmetric flows these methods are usually following a 1-D approach. The present work, proceeds one step further by examining the operation of a selective membrane, used for the decomposition of NH3, under a 2-D axissymetric CFD approach where the flow field, the chemical reactions and the selective porous membrane behaviour are being modeled and computed. The presence of the selective membrane was modeled as a porous medium with predetermined pressure drop and permeance behaniour. For this reason a structured computational grid was created and the flow field was computed as compressible, laminar and steady. At the inlet of the computational domain the mass flow was prescribed under the Hagen-Poiseuille profile and the static temperature was equal to 873K. The working fluid was a mixture of ammonia, hydrogen and nitrogen with prescribed mass fractions at the inlet of the computational domain. At the outlet the static pressure was set equal to ambient pressure. Due to the fact that the problem could be treated as axisymmetric only a cross section of the geometry was computed The main target of this effort was to obtain a more detailed view of the flow field and the calculation of the decomposition

of ammonia in comparison with previous 1-D modeling approaches and, thus, to evaluate the advantages and disadvantages of each method.

Back to program

Development of Advanced Polymerization Process Modeling, Simulation, Design and Optimization Tools Based on Interoperability Specifications

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As the polymer industry becomes more global and competitive, pressures are intensifying. European polymer manufacturers recognize that computer modeling is a key enabling technology in dealing with their current urgent needs regarding environment protection, cost reduction, product quality improvement, reduction of the time-to-market for new products, improved safety, global operation and competition. In fact, many of the current decisions in industry, regarding process design and operation, are being determined by solving deterministic or statistic optimization models with the aid of generic platforms equipped with optimization algorithms and enabling model developments with a structural architecture.

The development of software packages for the simulation of industrial polymerization processes requires a Computer Aided Design (CAD) expertise as an added value to the mathematical models of process units and physical properties evaluation. This expertise encompasses a wide variety of interdisciplinary fields such as numerical analysis, for the solution of differential and algebraic equations, mathematical programming, for the solution of optimization problems and computer science, in order to carry out the model developments exploiting the computer-technology capabilities offered today. The latter might imply qualifications that range from hardware, languages (FORTRAN, C++) and operating systems knowledge, up to programming approaches (mathematical modeling) and software structure skills (modular, equation-based approach, object-oriented programming).

The software structuring expertise and the state-of-the-art problem solving tools, although they are available to the major software vendors, they are the weak point of the individual modeling experts in the diverse fields of polymer process engineering. Most early process simulators were equipped their own process models, physical properties calculations, solvers and software design methods. However, there are strong incentives for moving from the traditional stand-alone software applications, to the development of software components, so that complete interoperability between different components from different process simulation environments can be achieved.

Our scope is the development of software packages in which the design of industrial polymerization processes will be based on an object-oriented programming environment. Based on this object-oriented programming design and the Cape Open (CO) specifications, the various structural elements of the polymerization process (e.g., materials, chemistry, unit operations, etc.) which describe the phenomena occurring in the micro-, meso- and macro- scales (e.g., polymerization kinetics, diffusion phenomena, phase equilibrium, mass and energy balances, etc.), can interact with other CO-compliant objects from different process modeling environments. Furthermore, an object-oriented designed process unit (e.g., PVC batch suspension polymerization reactor, high-pressure PE tubular reactor, etc.), will be capable to be exported and plugged in another process simulation environment in which it can be connected with other upstream and downstream equipment based on well-defined interfaces.

Back to program

Model-based Investigation of the Microbial Production of Polyhydroxyalcanoates (PHAs)

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Polyhydroxyalkanoates (PHAs) are microbial thermoplastics produced in a variety of micro-organisms as intracellular carbon and energy storage compounds. These compounds exhibit significant advantages over conventional polymeric materials as they are non-toxic, they come from renewable sources and they are 100% biodegradable. Polyhydroxybutyrate (PHB) constitutes the most important and widely studied representative of the PHAs. It is a biopolymer with mechanical properties similar to conventional commercial polymers like polypropylene or polyethylene. Therefore, PHB or its blends can potentially replace synthetic polymers in a variety of different applications. Despite the promise of these new materials, their introduction to the worldwide market is inhibited by a series of economic and engineering considerations. Commercially available biopolymers are at present, significantly more expensive than their synthetic alternatives. Therefore, there is an emerging need to reduce the overall cost of PHB production by designing novel processes and separation procedures in order to maximize its yield and productivity.

An attractive candidate microorganism for the production of PHB is the bacterium *Alcaligenes latus*. This specific bacterium exhibits certain advantages, as it utilizes a cheap substrate (i.e. sucrose) and accumulates PHB even during its growth phase with increased efficiency and selectivity. PHB is accumulated in the cytoplasm of *A. latus* as a membrane enclosed granule at a percentage up to 80-90% of the dry cell mass. The production rate/yield of PHB has been found to increase by imposing limitations on the nitrogen concentration in the presence of excess carbon source during non-growth conditions. Furthermore, yield and productivity of the PHB can be enhanced by eliminating the possible inhibition effect of the substrates on the specific growth rate of the microorganism.

In the present study a mathematical model was developed for the prediction of the dynamic evolution of the active biomass, substrates (i.e. carbon and nitrogen) and product (i.e. PHB) concentrations. In order to describe the specific growth rate of the micro-organism, different expressions available in literature were considered. Product formation was assumed to comprise growth and non-growth associated terms. Sucrose consumption was presumably due to the growth of catalytically active (residual) biomass, product formation and maintenance of the microorganism whereas nitrogen was consumed exclusively for the growth of the biomass.

Initially, the parameters of the model were adjusted using experimental data from batch and fed batch reactors. Subsequently, the effect of carbon and nitrogen levels on biomass growth and PHB accumulation in *A. latus* on a batch reactor was examined. The model was used to determine the optimal initial nitrogen-to-sucrose ratio and the composition of the culture medium, which correspond to the maximum PHB productivity. Finally, the model was applied for the simulation of an ideal fed-batch reactor system. Different feeding policies of the two substrates were examines in order to establish an optimal design strategy for the production of PHB.

Back to program

Analysis and a metabolic interpretation of the pH evolution during grape must alcoholic fermentation

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This work presents an analysis and a metabolic interpretation of the evolution of the pH during grape must alcoholic fermentation by Saccharomyces cerevisiae. The changes in the composition of the medium during fermentation are not enough to explain the variations of the pH observed in experiments. If the influence of the metabolism of ammoniac on the pH is well developed in the literature, the results are more dubious concerning the assimilation of the amino acids. In order to discriminate various assumptions, a model of pH calculation was developed. The pH is calculated by the resolution of a system of nonlinear algebraic equations consisted of the mass balances, chemical equilibriums and electro neutrality equation. The constant of dissociation of the organic acids is a function of alcohol and the temperature. The average activity coefficients are determined by the Debye-Hóckel law. An original formulation based on the concept of invariants of reaction made it possible to facilitate the initialization of the system. The model was validated on perfectly controlled synthetic mediums. The application of the model to fermentation media whose the nitrogen source is made up only of ammoniac gave very satisfactory results. It made it possible to explain the pH decrease observed by the assimilation of the nitrogen source. Once the exhausted nitrogen source, the increase in pH is directly related to the production of alcohol. The organic acids produced during fermentation exert only a very weak influence on the evolution of the pH. The use of the model made it possible to invalidate two assumptions concerning the impact of the assimilation of the amino acids on the pH. The most probable assumption is that the assimilation of the molecules of acids amino charged positively led to the emission of protons in the cellular extra medium.

Back to program

Energy Saving Potential of Phosphoric Acid Production by Wet Process

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Phosphoric acid production by wet method is economically preferable now days because there is low energy consumption and simple extractive purification of finished product in comparison with thermal method. In this work inspection of phosphoric acid concentration unit was done. Working process of the phosphoric acid production by dihydrate method is described. Process flowsheet analysis have shown low heat integration and heat transfer cross the pinch. Process integration methods application gives to reduce of energy consumption and improvement of environment situation. Process streams that may be included to heat integration were defined and analyzed. Material and heat balances of existing process were determined. Studying of heat recovery system allowed to define value of existing energy recuperation ~ 0.9 MW. It gives the possibility to build composite curves of existing process streams and to define hot utilities and cold utilities consumption. Application of process integration methods allow to increase recuperation of heat energy in existing process on 2.2 MW. Economic potential of energy saving in phosphoric acid production by wet process is 376 500 $. It makes 25% of heat energy consumption consumed today.

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Back to program

Dynamic Simulation and Control Studies of the Main Fractionation Column of a Heat Integrated Fluid Catalytic Cracking Plant

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Fluid catalytic cracking (FCC) is a process that has been commercially established for over 60 years; however, the technology continues to evolve to meet new challenges. The FCC process is very complex and involves interactive processes with constrained operating variables which are difficult to control, and the heat integration adds more complexity to the process itself. Hence, the overall economic benefits of a refinery could be considerably increased if proper control an optimization strategies are implemented. Previous studies of the process in dynamic state of a non-integrated FCC plant showed that the process can be optimized applying a more advanced control; however, the effect of the heat integration was not taken into account. Our objective is to evaluate the effect of the heat integration on the process, in dynamic state and under the effect of disturbances to be able to determine the best control strategy that assures the optimal performance of the process, in terms of heat recovery and final products quality. The system consists of a main column, LCO stripper, main column receiver, slurry settler, and the heat exchanger network (HEN) that integrates process streams from the gas concentration plant, and with the fresh feed stream to the FCC reactor. The system was simulated using ASPEN Plus and ASPEN DYNAMICS, the data used were provided by Rompetrol Oil Company and the HEN was analyzed using ASPEN HX-NET. The simulation results are in good agreement with the data provided and the products composition, evaluated in terms of their pseudo-components distribution, is in accordance with the experimental assays. So far, the heat integration analysis indicates that there is scope for improvement of the actual HEN that will be analyzed in terms of their controllability. Open-loop and close-loop response under the effect of disturbances (e.g., flow and temperature) were studied in order to identify the controllable and constraints variables. These results are very important in order to determine which advanced control technique (e.g, model predictive control, self-optimizing control) is best suited for the process.

Keywords: fluid catalytic cracking, dynamic simulation, heat integration.

Back to program

Study of a complex petrochemical process based on dynamical mathematical modeling analysis

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Studies concerned with the modeling of a complex industrial petrochemical process, namely Fluid Catalytic Cracking Unit, where made in order to elucidate the main characteristics of this unit dealing with strong interactions and many constraints from the operating, security and environmental point of view. By using dynamic mathematical modeling, it was developed a new simulator for this process, which was used for the study the dynamic behavior of the global reactor-regenerator-fractionator system, for the prediction of the pollutant gases emission (carbon monoxide) and also for the prediction of the composition of the main products (gasoline and diesel) in a wide range of operating conditions and in the presence of disturbances. The new FCCU developed model is sufficiently complex to capture the dynamic effects that occur in an actual FCCU system and is able to depict the main dynamic characteristics of a typical commercial FCC process. Simulations demonstrate the process is multivariable, strongly interacting and highly nonlinear. With the new simulator, economical aspects can be is also possible to investigate: the plant gross profit, pollutant gases emissions and gasoline octane number, in order to take logical decision concerning the increase in the plant profitability. The developed complex model is a very efficient tool to study and to improve the design, safe operation and performance of a modern complex petrochemical process.

Back to program

Application of Principal Component Analysis on a Hydrotreating Process

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Principal Component Analysis or PCA is a well-established technique for monitoring and disturbance detection of multivariate process, as it enables variability assessment through dimensionality reduction. PCA was applied to a hydroprocessing pilot plant to monitor the overall process variability. Contribution plots around points of increased variability were used to analyze process variability and its association with process variables. The methodology monitored successfully the set of 42 variables and diagnosed significant disturbances and their causes.

Back to program

The Simulation of Closed-loop Barometric Condenser System in Wet Phosphoric Acid Production Process

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In concentration stages of wet phosphoric acid production process for condensation of vapors from evaporation chamber usually are used contact type barometric condensers with open loop of cooling water. Such system makes some disadvantages: High consumption of fresh water is demanded; the big amount of water contaminated with fluorides and other substances with negative environment impact causes additive equipment capacities for water treatment; dependence of barometric condenser duty on water inlet temperature that may cause non-stable performance of condenser unit. The implementation of closed loop circulation system with heat exchanger as cooler of water circulated through barometric condenser will improve the situation. The use of high effective heat exchangers as water cooler is very important. The closed-loop barometric condenser system with plate and spiral heat exchangers is simulated for single-effect concentration unit in wet phosphoric acid production process. The basic demands for selection of heat exchangers were formulated. For simulation four types of plate heat exchangers and one type of spiral heat exchanger of Alfa Laval production were considered. Important criterion for plate-and-frame unit selection is possibility of mechanical cleaning of unit on place that causes the preference of single pass grouping. The appropriate software was developed. The selected types of plate-and-frame heat exchangers are discussed. For high contamination of solids the spiral heat exchanger as cooler is recommended.

Back to program

A non-linear MPC strategy for feed conversion targeting in a FCC pilot plant

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The main objective of this work is the development of an advanced control scheme for the Fluid Catalytic Cracking (FCC) Pilot Plant (PP) operated in the Chemical Process Engineering Research Institute (CPERI). This pilot plant is used for catalyst benchmarking, a very demanding procedure, that requires unit operation within a predefined span in order to match the industrial standards. For the tight, robust and efficient control of the FCC pilot plant a non-linear Model Predictive Control (MPC) strategy is implemented, along with an Extended Kalman Filter (EKF) for state and parameter estimation.

Back to program

The Impact of Product Lifecycle on Capacity Planning Best Policies of the Reverse Supply Chain with Remanufacturing

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Product recovery operations in reverse supply chains face rapidly changing demand due to the continuous changing demand and the increasing number of product offerings with reduced lifecycles. Therefore, the collection and remanufacturing capacity planning becomes a strategic issue of major importance for the profitability of closed-loop supply chains. The paper of Georgiadis, Vlachos and Tagaras (2006), developed through the methodology of System Dynamics, studies a closed-loop supply chain with remanufacturing and presents the results of dynamic capacity planning policies. The key issue of the paper is how the different lifecycles and return patterns of various products affect the optimal policies regarding expansion and contraction of collection and remanufacturing capacities. In this paper, various experiments are conducted so as to extract more specific conclusions about the robustness or sensitivity of those results. In particular, there are conducted 216 experiments that take under consideration various values of "peek demand", "failure percentage" of collected products that cannot be remanufactured and "reusable stock keeping time" of products that are profitable to be remanufactured, for every combination of the life cycle characteristics. The results of numerical examples with quite different lifecycle and return patterns show how the optimal collection and remanufacturing expansion/contraction policies depend on the lifecycle type and the average usage time of the product. The results also show that the collection and remanufacturing capacity policies are insensitive to the total product demand. The insensitivity of the optimal policies to total demand is a particularly appealing feature of the proposed model, given the difficulty in obtaining accurate demand forecasts.

Back to program

Generic Modelling, Design and Optimization of Industrial Phosphoric Acid Production Processes

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In the present work we address the systematic and effective design of industrial scale phosphoric acid production processes through the implementation of an efficient process modelling and optimization strategy. A generic and systematic framework is developed that aims to facilitate the modelling and identification of highly performing phosphoric acid production schemes through exploration of interactions and synergies among the participating processing components. The framework allows the employed models to be independent of the processes they are expected to emulate as it is developed through use of generic process modules, thus facilitating design variability and flowsheet interconnectivity. The employed modelling and optimization approach is implemented on an industrial phosphoric acid production process. Design options of increased performance are proposed for the existing process while useful design insights into the interactions of the process components are generated.

Keywords:
Phosphoric acid production, process design, cystallization process modelling

Back to program

Power Management Strategies on a Stand-Alone Power System Using Renewable Energy Sources and Hydrogen Storage

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A stand-alone power system based on a photovoltaic array and wind generators that stores the excessive energy from renewable sources in the form of hydrogen via water electrolysis for future use in a polymer electrolyte membrane fuel cell is currently being installed at Neo Olvio of Xanthi in Greece. The identification of efficient power management strategies (PMS) for the system has been performed through simulated experiments with anticipated conditions over a typical four months time period for the region of installation. The PMS have been assessed on their capacity to meet the load requirements under the fluctuations of the energy provided by the renewable energy sources (solar and wind) reliably and effective utilization of the electrolyzer and fuel cell. The key parameters in the PMS are the level of the energy provided by RES and the state of charge (SOC) of the accumulator. Hence, the operating policies for hydrogen production via water electrolysis and the fuel cell mainly depend on the excess or shortage of energy from the RES and the current level of SOC. A parametric sensitivity analysis has identified the influence of major parameters in the performance of the integrated system.

Keywords: Renewable Energy Sources, Stand-Alone Power System, PEM Electrolyzer, PEM Fuel Cell, Lead-Acid Accumulator, Hydrogen Production, Power Management Strategy

Back to program

Oil Production Optimization in Petroleum Reservoir

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The objective of the research presented in this paper is to investigate the effectiveness of a new stochastic algorithm to obtain maximum hydrocarbon production rate in petroleum reservoirs. The hydrocarbon production rate is function of several variables. Some of these variables are tubing diameter (which can be predictable by determining well radius), production well location, well flow pressure, injection well location and fluid injection rate. Changing any of the variables will alter the hydrocarbon production rate value. By using stochastic optimization techniques, there is no limit to the number of decision variables that can be optimized simultaneously. The presented method in this paper is a new metaheuristic algorithm which enables us to analyze a system of mathematical equations containing a large number of decision variables and determine the optimum values of them that should give the most economic result. This is referred to as Ant Colony Optimization algorithm. Ant Colony Optimization technique leads to lower computational cost to optimize complicated problems too. Although applied to discrete domains, this algorithm with some modifications has been applied to continuous optimization. Here, a numerical simulation is initially applied for modeling the hydrocarbon reservoir and then the results are analyzed and furthermore optimized to enhance profitability using Ant Colony Optimization algorithm. The developed code in MATLAB environment, based on Ant Colony Optimization, is able to estimate production and injection wells location, fluid injection rate, well radius and well flow pressure which would result in improved hydrocarbon production rate in two scenarios. This algorithm is simple to implement and the results of case studies show its ability to provide fast and accurate solutions. Results prove the reliability of algorithm for solving a large class of optimization problems in petroleum engineering.

Back to program