

12TH INTERNATIONAL SYMPOSIUM ON PROCESS SYSTEMS
ENGINEERING

&

25th EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS
ENGINEERING

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

Edited by

Krist V. Gernaey, Jakob K. Huusom and Rafiqul Gani

Department of Chemical and Biochemical Engineering

CAPEC-PROCESS Research Center

Technical University of Denmark

DK-2800 Lyngby, Denmark

Preface

It is our great pleasure to present this volume of Computer-Aided Chemical Engineering for the joint event of the 12th International Symposium on Process Systems Engineering (PSE) and the 25th European Symposium on Computer Aided Process Engineering (ESCAPE) in Copenhagen, Denmark. Through this conference we would like to highlight the contributions of the process systems engineering community to the sustainability of the modern society. Through contributions from academia and industry, we aim to establish the core products of PSE/CAPE, to point out the new and changing scope of our achievements, and to define the future challenges we face. We also would like to celebrate the 25th anniversary of the ESCAPE-series, the 12th PSE conference and the 39th year of the Computers and Chemical Engineering journal.

The PSE series is a triennial conference which has been held since 1982, organized on behalf of the international PSE Executive Committee with representations from countries from the Asia-Pacific, Europe and the Americas. The annual ESCAPE series started in Elsinore, Denmark in 1992 and is organized on behalf of the CAPE working party of the European Federation of Chemical Engineering. In 2006 these two events were also combined in Garmisch-Partenkirchen, Germany.

Both symposia serve as a forum for engineers, scientists, researchers, managers and students from academia and industry to report on progress that has been made in PSE/CAPE, to discuss the current challenges that need to be addressed, and, to highlight new developments in the applications of methods, algorithms, tools to solve a wide range of problems. The PSE-2015/ESCAPE-25 joint event includes a large number of keynote lecturers from industry and academia as well as four plenary lectures covering topics on globalization, energy, environment and health from well-known experts from all over the world. In addition close to 525 papers will be presented covering the following topics: modelling, numerical analysis and simulation; mathematical programming (optimization); cyber-infrastructure, informatics and intelligent systems; process and product synthesis/design; process dynamics, control and monitoring; abnormal events management and process safety; plant operations, integration, planning/scheduling and supply chain; enterprise-wide management and technology-driven policy making. As well as the following domain applications: molecular, biological, pharmaceutical, food, energy, and environmental systems engineering.

More than 1200 abstracts were submitted and the final technical program includes around 520 presentations out of which, 425 manuscripts are included in this proceedings volume. These manuscripts have been peer-reviewed and we thank the scientific committee members for their timely and thorough reviews. We would also like to thank our volunteers (Stefano Cignitti, Seyed S. Mansouri, Amata Anantpinijwatna, Maria-Ona Bertran, Rebecca Frauzem, Thomas Bisgaard and Xavi Flores-Alsina), without whose help this proceedings volume would not have been ready on time. Finally, we thank all the authors for their high quality manuscripts and for submitting them on time. We do hope the contents of this volume will serve as valuable reference to the scientific community and practitioners of systems engineering and a permanent record of the joint PSE-2015/ESCAPE-25 conference.

Krist V. Gernaey, Jakob K. Huusom & Rafiqul Gani
Department of Chemical & Biochemical Engineering
Technical University of Denmark, DK-2800 Lyngby, Denmark

7 March 2015

PSE2012/ESCAPE-25 Committees

Symposium Chair

Rafiqul Gani, Technical University of Denmark, Denmark

International Program Committee

- G. Henning, Universidad Nacional del Litoral, Argentina
- S. Diaz, PLAPIQUI, Argentina
- M. Narodoslawsky, Graz University of Technology, Austria
- F. Logist, University of Leuven, Belgium
- C. A. O. Nascimento, University of São Paulo, Brazil
- F. L. P. Pessoa, UFRJ, Rio de Janeiro, Brazil
- R. M. de Brito Alves, University of São Paulo, Brazil
- P. Stuart, École Polytechnique de Montréal, Canada
- L. Cisternes, Universidad de Antofagasta, Chile
- J. Wang, Sinopec, China
- J. Zhao, Tsinghua University, China
- F. Xiao, Xi'an Jiaotong University, China
- S. Zhang, IPE, Chinese Academy of Sciences, China
- K. M. Ng, Hong Kong University of Science and Technology, China (H.K.)
- K. Gernaey, Technical University of Denmark, Denmark
- J. K. Huusom, Technical University of Denmark, Denmark
- J. M. Woodley, Technical University of Denmark, Denmark
- B.-G. Rong University of Southern Denmark, Denmark
- S. Pierucci, Politecnico di Milano, Italy
- F. Bezzo, University of Padova, Italy
- S. Hasebe, Kyoto University, Japan
- M. Hirao, University of Tokyo, Japan
- Y. Yamashita, Tokyo University of Agriculture and Technology, Japan
- M. Kano, Kyoto University, Japan
- Y. Fukui, Mitsubishi Chemical Corporation, Japan
- I.-B. Lee, Pohang University of Science and Technology, Korea
- I. Moon, Yonsei University, Korea
- J. H. Lee, KAIST, Korea
- C. Han, Seoul National University, Korea
- D. Foo, University of Nottingham, Malaysia
- Z. A. Manan, Universiti Teknologi Malaysia, Malaysia
- M. Sales-Cruz, Universidad Autónoma Metropolitana-Cuajimalpa, Mexico
- A. Jimenez Instituto Tecnológico de Celaya, Mexico
- E. Perez-Cisneros, Universidad Autónoma Metropolitana, Mexico
- S. Skogestad, Norwegian University of Science and Technology, Norway
- A. Barbosa- Póvoa, Technical University of Lisbon, Portugal
- J. V. Schijndel, Shell International Chemicals, The Netherlands
- A. J. B. ten Kate, AkzoNobel Chemicals B.V., The Netherlands
- M. Turkay, Koc University, Turkey
- E .N. Pistikopoulos, Imperial College London, UK
- C. C. Pantelides, PSE Enterprise, UK
- P. Piccione, Syngenta Ltd., UK
- A. Azapagic, University of Manchester, UK
- I. D. L. Bogle, University College London, UK
- G. V. Reklaitis, Purdue University, USA
- L. Biegler, Carnegie Mellon University, USA
- I. E. Grossmann, Carnegie Mellon University, USA
- V. Venkatasubramanian, Columbia University, USA
- M. Ierapetritou, Rutgers University, USA
- A. Linninger, University of Illinois at Chicago, USA
- M. R. Eden, Auburn University, USA
- C. A. Floudas, Princeton University USA
- Z. Nagy, Purdue University, USA
- Y. Huang, Wayne State University, USA

- B. Sarup, Alfa Laval
Copenhagen, Denmark
- P. M. Harper, Harper & Vedel
Denmark
- X. Joulia, INP-ENSIACET,
France
- J. M. Le Lann, INP-
ENSIACET, France
- S. Engell, Technical University
of Dortmund, Germany
- J. Kussi, Bayer AG, Germany
- A. Bode, BASF AG, Germany
- I. Harjunkoski, ABB, Germany
- P. Lutze, Technical University
of Dortmund, Germany
- A. C. Kokossis, National
Technical University of Athens,
Greece
- F. Friedler, University of
Pannonia, Hungary
- J. Klemes, University of
Pannonia, Hungary
- S. Munawar, Indian Institute of
Technology Delhi, India
- M. Bhushan, Indian Institute of
Technology Bombay, India
- R. Srinivasan, Indian Institute of
Technology Gandhinagar, India
- N. Mostoufi, University of
Tehran, Iran
- H. Matos, Universidade de
Lisboa, Portugal
- N. ElBashir, Texas A&M
University at Qatar, Qatar
- S. Agachi Babes-Bolyai,
University, Romania
- N. Menshutina, D. Mendeleev
University of Chemical
Technology of Russia, Russia
- I. A. Karimi, National
University of Singapore,
Singapore
- Z. Kravanja, University of
Maribor, Slovenia
- D. Hildebrandt, University of
the Witwatersrand, South Africa
- T. Majози, University of the
Witwatersrand, South Africa
- L. Puigjaner, University
Politecnica de Catalunya, Spain
- A. Espuña, Universidad
Politecnica de Catalunya, Spain
- F. Marechal, École
Polytechnique Fédérale de
Lausanne, Swiss
- C.-L. Chen, National Taiwan
University, Taiwan
- P. Kittisupakorn, Chulalongkorn
University, Thailand
- A. Kammafoo, SCG Chemicals,
Thailand
- R. Meier, DSM, The
Netherlands
- M. El-Halwagi, Texas A&M
University, USA
- L. Achenie, Virginia
Polytechnic Institute & State
University, USA
- J. J. Siirola, Carnegie Mellon
University/Purdue University,
USA
- C. T. Maravelias, University of
Wisconsin-Madison, USA
- N. Sahinidis, Carnegie Mellon
University, USA
- M. Bassett, Dow AgroSciences
LLC, USA
- B. Wayne Bequette, Rensselaer
Polytechnic Institute, USA
- K. C. Furman, Exxon, USA
- M. K. Burka, NSF, USA
- Fengqi You, Northwestern
University, USA
- C. Gonzalez-Jimenez, GSK,
USA
- S. Balakrishna, Optience, USA
- I-L. Chien, National Taiwan
University, Taiwan

Local Organizing Committee (Technical University of Denmark, Denmark)

Rafiqul Gani
John M. Woodley
Krist V. Gernaey
Ulrich Krühne
Jakob K. Huusom

Eva Mikkelsen
Maria-Ona Bertran
Rebecca Frauzem
Stefano Cignitti
Seyed S. Mansouri

Amata Anantpinijwatna
Thomas Bisgaard
Deenesh K. Babi
Xavi Flores-Alsina

Sponsors

Gold Sponsors



HEMPEL



COWIfonden



Silver Sponsors



Bronze sponsors

syngenta



Table of Contents

Preface

Committees

Sponsors

Plenary Papers

Recent advances in mathematical programming techniques for the optimization of process systems under uncertainty <i>Ignacio E. Grossmann, Robert M. Apap, Bruno A. Calfa, Pablo Garcia-Herreros, Qi Zhang</i>	1
A multidisciplinary hierarchical framework for the design of consumer centered chemical products <i>Ka M. Ng</i>	15
Multi-Level design of process systems for efficient chemicals production and energy conversion <i>Kai Sundmacher</i>	25
Keynote Papers	
PSE tools for process intensification <i>Philip Lutze</i>	35
Towards the integration of process design, control and scheduling: Are we getting closer? <i>Efstathios N. Pistikopoulos, Nikolaos A. Diangelakis, Amit M. Manthanwar</i>	41
Industrially applied PSE for problem solving excellence <i>Antoon J. B. ten Kate</i>	49
Sustainable production of liquid fuels <i>Jonathan P. Raftery, M. Nazmul Karim</i>	55
Industrial perspectives on deployment of scheduling solutions <i>Iiro Harjunkoski</i>	63
Overview of smart factory studies in petrochemical industry <i>Defang Li, Baihua Jiang, Hansheng Suo, Ya Guo</i>	71
A PSE approach to patient-individualized physiologically based pharmacokinetic modeling <i>Roberto A. Abbiati, Gaetano Lamberti, Anna A. Barba, Mario Grassi, Davide Manca</i>	77
Modeling and optimization of continuous pharmaceutical manufacturing processes <i>Amanda Rogers, Marianthi Ierapetritou</i>	85
Process technology licensing: An interface of engineering and business <i>Andreas Bode, Jose Castro-Arce, Bernd Heida, Carsten Henschel, Achim Wechsung</i>	93
Simple rules for economic plantwide control <i>Vladimiro Minasidis, Sigurd Skogestad, Nitin Kaistha</i>	101
Mixed-Integer fractional programming: Models, algorithms, and applications in process operations, energy systems, and sustainability <i>Fengqi You</i>	109
Advances and challenges in modelling of processing of lipids <i>Bent Sarup</i>	117
A perspective on PSE in fermentation process development and operation <i>Krist V. Gernaey</i>	123
Sustainable production and consumption: A decision-support framework based on a systems approach to integrating environmental, economic and social aspects of sustainability <i>Adisa Azapagic</i>	131

Control of reaction systems via rate estimation and feedback linearization 137
Diogo Rodrigues, Julien Billeter, Dominique Bonvin

Modeling the fixed-bed Fischer-Tropsch reactor in different reaction media 143
Rehan Hussain, Jan H. Blank, Nimir O. Elbashir

Contributed Papers

T-0: PSE-CAPE and Education

Process simulators: What students forget when using them, their limitations, and when not to use them 149
Joseph A. Shaeiwitz, Richard Turton

Learning to solve mass balance problems through a web-based simulation environment 155
Alexandros Koulouris, Dimitrios Vardalis

Model predictive control of post-combustion CO₂ capture process integrated with a gas-fired power plant 161
Evgenia D. Mechleri, Niall Mac Dowell, Nina F. Thornhill

A framework to structure operational documents for chemical processes 167
Hiroshi Osaka, Yuji Naka, Tetsuo Fuchino

Teaching sustainable process design using 12 systematic computer-aided tasks 173
Deenesh K. Babi

Contributed Papers

T-1: Modelling, Numerical Analysis and Simulation

Optimization of chemical processes using surrogate models based on a kriging interpolation 179
Natalia Quirante, Juan Javaloyes, Rubén Ruiz-Femenia, José A. Caballero

Global sensitivity analysis for a model of B-Cell chronic lymphocytic leukemia disease trajectories 185
Symeon V. Savvopoulos, Ruth Misener, Nicki Panoskaltzis, Efstratios N. Pistikopoulos, Athanasios Mantalaris

Modelling and simulation of complex nonlinear dynamic processes using data based models: application to photo-fenton process 191
Ahmed Shokry, Francesca Audino, Patricia Vicente, Gerard Escudero, Montserrat Perez Moya, Moisès Graells, Antonio Espuña

A meshfree maximum entropy method for the solution of the population balance equation 197
Menwer Attarakih, Abdelmalek Hasseine, Hans-Jörg Bart

Modelling the hydrodynamics of bubble columns using coupled OPOSPM-maximum entropy method 203
Menwer Attarakih, Ferdaous Al-Slaihata, Mark W. Hlawitschkac, Hans-Jörg Bart

Process simulation of a 420MW gas-fired power plant using Aspen Plus 209
Bao-Hong Li, Nan Zhang, Robin Smith

Optimal blending study for the commercial gasoline 215
Cristian Patrascioiu, Doicin Bogdan, Grigore Stamatescu

Population balance model for enzymatic depolymerization of branched starch 221
Christoph Kirse, Heiko Briesen

Analysis of the transfer of radical copolymerization systems from semi-batch to continuous plants 227
Thilo Goerke, Sebastian Engell

Thermodynamic considerations for systems biocatalysis 233
Rohana Abu, Maria T. Gundersen, John M. Woodley

Parallel computation method for solving large scale equation-oriented models 239
Yannan Ma, Jinzu Weng, Zhijiang Shao, Xi Chen, Lingyu Zhu, Yuhong Zhao

Dynamic investment appraisal: Economic analysis of mobile production concepts in the process industry <i>Gerben Bas, Telli E. Van der Lei</i>	245
Prediction heat capacity of ionic liquids based on COSMO-RS $S\sigma$ -profile <i>Yongsheng Zhao, Ying Huang, Xiangping Zhang, Suojiang Zhang</i>	251
OPOSSIM: A population balance-SIMULINK module for modelling coupled hydrodynamics and mass transfer in liquid extraction equipment <i>Menwer Attarakih, Samer Al-Zyod, Mark Hlawitschke, Hans-Jörg Bart</i>	257
CFD-DEM simulation of a fluidized bed crystallization reactor <i>Kristin Kerst, Luis M. de Souza, Antje Bartz, Andreas Seidel-Morgenstern, Gábor Janiga</i>	263
A modelling, simulation, and validation framework for the distributed management of large-scale processing systems <i>Shaghayeg Nazari, Christian Sonntag, Goran Stojanovski, Sebastian Engell</i>	269
Performance analysis and optimization of the biomass gasification and Fischer-Tropsch integrated process for green fuel Productions <i>Karittha Im-orb, Lida Simasatitkul, Amornchai Arpornwichanop</i>	275
Dynamic behavior adjustment of 1, 3-propanediol fermentation process <i>Hao Jiang, Nan Zhang, Jinsong Zhao, Tong Qiu, Bingzhen Chen</i>	281
Modelling and simulation of pressure swing adsorption (PSA) processes for post-combustion carbon dioxide (CO ₂) capture from flue gas <i>George N. Nikolaidis, Eustathios S. Kikkinides, Michael C. Georgiadis</i>	287
Validation of a functional model for integration of safety into process system design <i>Jing Wu, Morten Lind, Xinxin Zhang, Sten Bay Jørgensen, Gürkan Sin</i>	293
A dynamic method for computing thermodynamic equilibria in process simulation <i>Alexander Zinser, Kongmeng Ye, Liisa Rihko-Struckmann, Kai Sundmacher</i>	299
Dynamics and operation analysis of the PHB (polyhydroxybutyrate) fermentation <i>Moises González-Contreras, Omar Anaya-Reza, Mauricio Sales-Cruz, Teresa Lopez-Arenas</i>	305
Retrofitting of concentration plants using global sensitivity analysis <i>Freddy Lucay, Luis A. Cisternas, Edelmira D. Gálvez</i>	311
Differential-algebraic approach to solve steady-state two-phase flow drift-flux model with phase change <i>Rodrigo G. D. Teixeira, Argimiro R. Secchi, Evaristo C. Biscaia Jr.</i>	317
Model-based design of experiments for the identification of kinetic models in microreactor platforms <i>Federico Galvanin, Enhong Cao, Noor Al-Rifai, Asterios Gavriilidis, Vivek Dua</i>	323
Application of derivative - free estimator for semi batch autocatalytic esterification reactor: Comparison study of unscented Kalman filter, divided difference Kalman filter and cubature Kalman <i>Fakhrony S. Rohman, Suhairi A. Sata, Norashid Aziz</i>	329
Modeling and parameter estimation of coke combustion kinetics in a glycerol catalytic conversion reactor <i>Minghai Lei, François Lesage, M. Abderrazak Latifi, Serge Tretjak</i>	335
Behavior of heavy metals during gasification of phytoextraction plants: thermochemical modelling <i>Marwa Saïd, Laurent Cassayre, Jean-Louis Dirion, Ange Nzihou, Xavier Joulia</i>	341
Multi-objective optimization for the production of fructose in a Simulated Moving Bed Reactor <i>Edwin Zondervan, Bram van Duin, Nikola Nikacevic, Jan Meuldijk</i>	347
A modeling framework for optimal design of renewable energy processes under market uncertainty <i>Aryan Geraili, Jose A. Romagnoli</i>	353

A molecular reconstruction feed characterization and CAPE OPEN implementation strategy to develop a tool for modeling HDT reactors for light petroleum cuts <i>César G. Pernaleté, Jasper van Baten, Juan C. Urbina, José F. Arévalo</i>	359
Techno-economic analysis of ethanol-selective membranes for corn ethanol-water separation <i>Adam Kelloway, Michael Tsapatsis, Prodromos Daoutidis</i>	365
Equation-oriented modeling of multi-stream heat exchanger in air separation units <i>Liuzhen Jiang, Kai Zhou, Lingyu Zhu</i>	371
Proposal of a new pathway for microalgal oil production and its comparison with conventional method <i>Sofia Chaudry, Parisa A. Bahri, Navid R. Moheimani</i>	377
Superstructure development, simulation and optimization of desalination systems using Aspen Custom modeler <i>Sidra N. Malik, Parisa A. Bahri, Linh T. T. Vu</i>	383
Microalgae growth determination using breakage equation model <i>Ergys Pahija, Yu Zhang, Moojian Wang, Yi Zhu, Chi W. Hui</i>	389
A new strategy for the simulation of gas pipeline network based on system topology identification <i>Zengzhi Du, Chunxi Li, Wei Sun, Jianhong Wang</i>	395
Modelling and optimization of a heat integrated gasification process <i>Yi Zhu, Adetoyese O. Oyedun, Maojian Wang, Ergys Pahija, Chi W. Hui</i>	401
Analyzing and modeling ethylene cracking process with complex networks approach <i>Fang Zhou, Qiu Tong, Bingzhen Chen</i>	407
Optimization and economic evaluation of bioethanol recovery and purification processes involving extractive distillation and pressure-swing adsorption <i>Yoke Y. Loy, Xin L. Lee, Gade P. Rangaiah</i>	413
Data reconciliation in reaction systems using the concept of extents <i>Sriniketh Srinivasan, Julien Billeter, Shankar Narasimhan, Dominique Bonvin</i>	419
Development of a generic model of a Ruthenium reactor <i>Norbertin N. Eyeghe, Carl Sandrock, Carel Van Dam</i>	425
Dynamic modelling and experimental validation of a pilot-scale tubular continuous reactor for the autohydrolysis of lignocellulosic materials <i>Carlos González-Figueroa, Arturo Sánchez, German Díaz, Felicia Rodríguez, Roberto Flores, Marco A. Ceballos, Ramón Puente, Héctor A. Ruiz</i>	431
First-principles model diagnosis in batch systems by multivariate statistical modeling <i>Natascia Meneghetti, Pierantonio Facco, Sean Bermingham, David Slade, Fabrizio Bezzo, Massimiliano Barolo</i>	437
Integrated analysis of an evaporation and distillation bioethanol industrial system using direct and indirect heating <i>Rodrigo O. Silva, Vandr�e C. Tiski, Rafael O. Defendi, Lucas B. Rocha, Oswaldo C. M. Lima, Laureano Jim�enez, Luiz M. M. Jorge</i>	443
Reformulating the minimum eigenvalue maximization in optimal experiment design of nonlinear dynamic biosystems <i>Dries Telen, Nick Van Riet, Filip Logist, Jan Van Impe</i>	449
A framework for modular modeling of the diesel engine exhaust gas cleaning system <i>Andreas �berg, Thomas K. Hansen, Kasper Linde, Anders K. Nielsen, Rune F. Damborg, Anders Widd, Jens Abildskov, Anker D. Jensen, Jakob K. Huusom</i>	455
An approximate modeling method for industrial L-lysine fermentation process <i>Hangzhou Wang, Faisal Khan, BoChen, Zongmei Lu</i>	461

Model-based prediction and experimental validation of viscosities of soap emulsions <i>Daniel M. Macías-Pelayo, Pedro A. Alonso-Dávila, Alfonso Martínez-Villalobos, Alicia Román-Martínez</i>	467
A novel quantisation-based integration method for ODEs <i>Vassilios S. Vassiliadis, Fabio Fiorelli, Harvey Arellano-Garcia</i>	473
Modeling and parameter estimation of enzymatic biodiesel synthesis <i>Priscila S. Sabaini, Thais F. C. Salum, Rossano Gambetta, Fabricio Machado</i>	479
Analysis of two alternatives to produce ethylene from shale gas <i>Andrea P. Ortiz-Espinoza, Mahmoud M. El-Halwagi, Arturo Jiménez-Gutiérrez</i>	485
A crude oil econometric model for PSE applications <i>Davide Manca, Valentina Depetri, Clément Boisard</i>	491
Simulation study of temperature distribution in the thermal drying oven for a lacquer coating process <i>Paisan Kittisupakorn, Patsarawan Lipikanjanakul</i>	497
Estimation and uncertainty analysis of flammability properties of chemicals using group-contribution property models <i>Jérôme Frutiger, Jens Abildskov, Gürkan Sin</i>	503
Integration and optimization of an air separation unit (ASU) in an IGCC plant <i>Maojian Wang, Adetoyese O. Oyedun, Ergys Pahija, Yi Zhu, Guilian Liu, Chi W. Hui</i>	509
Mathematical modeling of an industrial delayed coking unit <i>Claudio N. Borges, Maria A. Mendes, Rita M. B. Alves</i>	515
Post-combustion CO ₂ capture with sulfolane based activated alkanolamine solvent <i>Sukanta K. Dash, Bikash K. Mondal, Amar N. Samanta, Syamalendu S. Bandyopadhyay</i>	521
Modeling and sensitivity analysis of a medium-temperature gas cleaning process of biogenous synthesis gas <i>Michaela Fraubaum, Heimo Walter</i>	527
Exergy analysis of monoethylene glycol (MEG) recovery systems <i>Alexandre M. Teixeira, José L. de Medeiros, Ofélia Q. F. Araújo</i>	533
Production of biodiesel via enzymatic palm oil ethanolysis: Kinetic study <i>Shayane P. Magalhães, Fernando L. P. Pessoa, Tito L. M. Alves</i>	539
Integration of retrofitted coal-fired power plant with CCS: Power derate minimization <i>Jinjoo An, Ung Lee, Jaeheum Jung, Chonghun Han</i>	545
CUDA-optimized cellular automata for diffusion limited processes <i>Andrey Kolnoochenko, Natalia Menshutina</i>	551
Effect of ship motion on amine absorber with structured-packing for CO ₂ removal from natural gas: An approach based on porous medium CFD model <i>Dung A. Pham, Young-Il Lim, Hyunwoo Jee, Euisub Ahn, Youngwon Jung</i>	557
Model-based analysis and efficient operation of a glucose isomerization reactor plant <i>Emmanouil Papadakis, Ulrich Madsen, Sven Pedersen, Krist V. Gernaey, John M. Woodley, Rafiqul Gani</i>	563
pyIDEAS: An open-source python package for model analysis <i>Timothy Van Daele, Stijn Van Hoey, Ingmar Nopens</i>	569
A numerical procedure for model identifiability analysis applied to enzyme kinetics <i>Timothy Van Daele, Stijn Van Hoey, Krist V. Gernaey, Ulrich Krühne, Ingmar Nopens</i>	575
Integrated simulation platform of chemical processes based on virtual reality and dynamic model <i>Na Luo, Xiaoqiang Wang, Feng Van, Zhen-Cheng Ye, Feng Qian</i>	581

OsmoseLua - An integrated approach to energy systems integration with LCIA and GIS <i>Min-Jung Yoo, Lindsay Lessard, Maziar Kermani, François Maréchal</i>	587
Incremental kinetic identification based on experimental data from steady-state plug flow reactors <i>Nirav Bhatt, Srividhya Visvanathan</i>	593
Nonlinear fuzzy identification of batch polymerization processes <i>Nádson N. M. Lima, Lamia Z. Linan, Delba N. C. Melo, Flavio Manenti, Rubens M. Filho, Marcelo Embiruçu, Maria R. Wolf Maciel</i>	599
Modeling dissolution of solids based on cellular automata with changing sizes of cells <i>Sviatoslav I. Ivanov, Irina A. Tiptsova, Natalia V. Menshutina</i>	605
Data analysis and modelling of a fluid catalytic cracking unit (FCCU) for an implementation of real time optimization <i>Juan D. Reyes, Adriana L. Rodriguez, Carlos A. M. Riascos</i>	611
A hybrid discrete/continuous dynamic model of trayed tower hydraulics <i>David Pinilla-García, Santos Galán</i>	617
application of the lagrangian cfd approach to modelling of crystallization in stirred batch reactors using the smoothed particle hydrodynamics method <i>Dragan D. Nikolic, Brian P. de Souza, Patrick J. Frawley</i>	623
Model reduction in visual modelling <i>Heinz A. Preisig</i>	629
Automatic reconstruction and generation of structured hexahedral mesh for non-planar bifurcations in vascular network <i>Mahsa Ghaffari, Chih-Yang Hsu, Andreas A. Linninger</i>	635
Developing surrogate models via computer-based experiments <i>Mandar N. Thombre, Heinz A. Preisig, Misganaw B. Addis</i>	641
Systematic development of kinetic models for systems described by linear reaction schemes <i>Carolina S. Vertis, Nuno M. C. Oliveira, Fernando P. M. Bernardo</i>	647
Rigorous modeling, simulation and optimization of a dividing wall batch reactive distillation column: A comparative study <i>Edna S. Lopez-Saucedo, Juan G. Segovia-Hernandez, Ignacio E. Grossmann, Salvador Hernandez-Castro</i>	653
Theoretical modeling of (bases) reactive residue curve maps for tame synthesis system using Matlab – simulis thermodynamics communication facilities <i>M. M. Ceaşescu, Jordi Bonet-Ruiz, V. Pleşu, A. E. Iancu, A. E. Bonet-Ruiz</i>	659
Alternative prediction models for data scarce environment <i>Ali Al-Shanini, Arshad Ahmad, Faisal Khan, Olagoke Oladokum, Shadia H. M. Nor</i>	665
Multi-objective optimisation of atmospheric crude distillation system operations based on bootstrap aggregated neural network models <i>Funmilayo N. Osulale, Jie Zhang</i>	671
Optimization studies through simulation of a methanol/water/glycerol distillation column <i>José Palmeira, João M. Silva, Henrique A. Matos</i>	677
Simulation of a 3D bioprinted human vascular segment <i>J. A. Nogueira, V. F. Lara, T. S. Marques, D. S. Oliveira, V. Mironov, J. V. da Silva, R. A. Rezende</i>	683
Modeling fixed-bed multicomponent adsorption as a step to achieve ultra-low sulfur diesel <i>Tristán Esparza-Isunza, Felipe Lopez-Isunza</i>	689

Experimental and CFD simulation studies of circulating fluidized bed riser in the fast fluidization regime	695
<i>Mukesh Upadhyay, Myung W. Seo, Nam S. Nho, Jong-Ho Park</i>	
Application of new electrolyte model to phase transfer catalyst (PTC) systems	701
<i>Sun H. Kim, Amata Anantpinijwatna, Jeong-Won Kang, Mauricio Sales-Cruz, Rafiqul Gani</i>	
A novel rigorous mathematical programming approach to construct phenomenological models	707
<i>Vassilios S. Vassiliadis, Yian Wang, Harvey Arellano-Garcia, Ye Yuan</i>	
Dynamic simulation of a batch aqueous two-phase extraction process for α -amylase	713
<i>Nehal Patel, Daniel G. Bracewell, Eva Sorensen</i>	
Contributed Papers	
T-2: Mathematical Programming (Optimization)	
A framework for hybrid multi-parametric model-predictive control with application to intravenous anaesthesia	719
<i>Ioana Nascu, Richard Oberdieck, Efstratios N. Pistikopoulos</i>	
Dynamic chance-constrained optimization under uncertainty on reduced parameter sets	725
<i>David Müller, Erik Esche, Sebastian Werk, Günter Wozny</i>	
Optimal design of thermal membrane distillation networks	731
<i>Ramon González-Bravo, Fabricio Nápoles-Rivera, José María Ponce-Ortega, Medardo Serna-Gonzalez, Mahmoud El-Halwagi</i>	
Multicolumn-multicut cross decomposition for stochastic mixed-integer linear programming	737
<i>Emmanuel Ogbe, Xiang Li</i>	
Efficient ant colony optimization (EACO) for solvent selection using computer aided molecular design	743
<i>Berhane H. Gebreslassie, Urmila M. Diwekar</i>	
Optimisation of process parameters with simultaneous consideration of energy efficiency measures	749
<i>Timo Bohnenstaedt, Kristina Zimmermann, Georg Fieg</i>	
Optimization of split fractions and cleaning schedule management in heat exchanger networks	755
<i>Jian Du, Jie Fan, Linlin Liu, Jilong Li, Yu Zhuang, Quinwei Meng</i>	
A cost targeting method for estimating investment on heat exchanger networks for collection of industrial excess heat	761
<i>Matteo Morandin, Lina Eriksson</i>	
Ellipsoidal arithmetic for multivariate systems	767
<i>Mario E. Villanueva, Jai Rajyaguru, Boris Houska, Benoît Chachuat</i>	
Reduced model trust region methods for embedding complex simulations in optimization problems	773
<i>John P. Eason, Lorenz Biegler</i>	
Optimization of LNG supply chains	779
<i>Alice Bittante, Raine Jokinen, Frank Pettersson, Henrik Saxén</i>	
Metaheuristic techniques for the optimal design of ngl pipelining	785
<i>Paola P. Oteiza, Martín C. De Meio Reggiani, Diego A. Rodriguez, Valentina Viego, Nélide B. Brignole</i>	
Deterministic global dynamic optimisation using interval analysis	791
<i>Carlos Perez-Galvan, I. David L. Bogle</i>	
Separation process optimization under uncertainty by chance constraint programming with recourse	797
<i>Li Sun, Huajie Zhang</i>	
Optimal operating policies for synthesizing tailor made gradient copolymers	803
<i>Cecilia Fortunatti, Bruno M. Mato, Adriana Brandolin, Claudia Sarmoria, Mariano Asteasuain</i>	

Degeneracy hunter: an algorithm for determining irreducible sets of degenerate constraints in mathematical programs	809
<i>Alexander W. Dowling, Lorenz T. Biegler</i>	
Dynamic multi-objective optimization of batch chromatographic separation processes	815
<i>Anders Holmqvist, Fredrik Magnusson, Bernt Nilsson</i>	
An adaptive multi-objective differential evolution algorithm for solving chemical dynamic optimization problems	821
<i>Xu Chen, Wenli Du, Feng Qian</i>	
Optimal operation of a pyrolysis reactor	827
<i>Aysar T. Jarullah, Shema A. Hameed, Zina A. Hameed, Iqbal M. Mujtaba</i>	
Representation of the convex envelope of bilinear terms in a reformulation framework for global optimisation	833
<i>Andreas Lundell, Tapio Westerlund</i>	
Interactive multi-objective decision-support for the optimization of nonlinear dynamic (bio)chemical processes with uncertainty	839
<i>Mattia Vallerio, Jan Hufkens, Jan Van Impe, Filip Logist</i>	
Superstructure optimisation of a water minimization network with an embedded multi-contaminant electro dialysis model	845
<i>Chiedza D. Nezungai, Thokozani Majosi</i>	
Deterministic global optimization and transition states	851
<i>Dimitrios Nerantzis, Claire S. Adjiman</i>	
A metaheuristic for solving large-scale two-stage stochastic mixed 0-1 programs with a time consistent stochastic dominance constraints risk averse strategy	857
<i>Susana Baptista, Ana P. Barbosa-Póvoa, Laureano Escudero, Maria I. Gomes, Celeste Pizarro</i>	
Optimized production of multilayered monodisperse polymer nanoparticles	863
<i>Brahim Benyahia, M. Abderrazak Latifi, Christian Fonteix, Fernand Pla</i>	
Systematic design of chemical reactors with multiple stages via multi-objective optimization approach	869
<i>Mohd N. Mohd Fuad, Mohd A. Hussain</i>	
Synthesis and design of integrated process and water networks	875
<i>Zainatul B. Handani, Alberto Quaglia, Rafiqul Gani</i>	
Optimization of high-density polyethylene slurry process based on molecular weight distribution and chemical composition distribution under uncertainty	881
<i>Jiayuan Kang, Xi Chen, Zhijiang Shao</i>	
A systematic approach for targeting zero liquid discharge in industrial parks	887
<i>Zakarya A. Othman, Patrick Linke, Mahmoud El-Halwagi</i>	
Decomposition techniques for the real-time optimization of a propylene production unit	893
<i>Alvaro Marcelo Acevedo Peña, José Eduardo Alves Graciano, Fabio dos Santos Liporace, Ardson dos Santos Vianna Jr., Galo Antonio Carrillo Le Roux</i>	
An approach to deal with non-convex models in real-time optimization with modifier adaptation	899
<i>Maximiliano Garcia, Juan Pablo Ruiz, Marta Basualdo</i>	
A robust minimax Semidefinite Programming formulation for optimal design of experiments for model parameterisation	905
<i>Belmiro P. M. Duarte, Guillaume Sagnol, Nuno M. C. Oliveira</i>	
Design of a multi-contaminant water allocation network using multi-objective optimization	911
<i>Sofía D. Almaraz, Marianne Boix, Catherine Azzaro-Pantel, Ludovic Montastruc, Serge Domenech</i>	

Simulation and optimization of the ethane cracking process to produce ethylene <i>Daison Y. Caballero, Lorenz T. Biegler, Reginaldo Guirardello</i>	917
Study of performance of a novel stochastic algorithm based on Boltzmann distribution (BUMDA) coupled with self-adaptive handling constraints technique to optimize chemical engineering process <i>Rodolfo Murrieta-Dueñas, Jazmin Cortez-González, Arturo Hernández-Aguirre, Roberto Gutiérrez-Guerra, Salvador Hernandez, Juan G. Segovia Hernández</i>	923
Dynamic modelling and optimal design of the solid-phase reactive chromatographic separation system for biomass saccharification via acid hydrolysis <i>Pakkapol Kanchanalai, Matthew J. Realff, Yoshiaki Kawajiri</i>	929
Contributed Papers	
T-3: Cyber-Infrastructure, Informatics and Intelligent Systems	
Life cycle simulation for a process plant based on a two-dimensional co-simulation approach <i>Mathias Oppelt, Gerrit Wolf, Leon Urbas</i>	935
On the process of building a process system engineering ontology using a semi-automatic construction approach <i>Canan Dombayci, Javier Farreres, Horacio Rodríguez, Edrisi Muñoz, Elisabet Capón-García, Antonio Espuña, Moisés Graells</i>	941
Graphical processing unit (GPU) accelerated solution of multi-dimensional population balances using high resolution finite volume algorithm <i>Botond Szilagy, Zoltan K. Nagy</i>	947
Development of computer aided modelling templates for model re-use in chemical and biochemical process and product design: import and export of models <i>Marina Fedorova, Gregor Tolksdorf, Sandra Fillinger, Günter Wozny, Mauricio Sales-Cruz, Gürkan Sin, Rafiqul Gani</i>	953
BiOnto: An Ontology for biomass and biorefining technologies <i>Nikolaos Trokanas, Madeleine Bussemaker, Eirini Velliou, Hella Tokos, Franjo Cecelja</i>	959
Linking process, electrical and logical connectivity for supported fault diagnosis <i>David Dorantes Romero, Tone-Grete Graven, Nina F. Thornhill</i>	965
An interactive framework for building and analysing models of urban energy systems <i>Kamal Kuriyan</i>	971
Model-based analysis of waste management systems through a natural language approach <i>Vasileios Magioglou, Elisabet Capón-García, Sara Badr, Antonis Kokossis</i>	977
Enterprise-wide scheduling framework supported by knowledge management <i>Elisabet Capón-García, Edrisi Muñoz, José M. Laínez-Aguirre, Antonio Espuña, Luis Puigjaner</i>	983
Knowledge management to support the integration of scheduling and supply chain planning using Lagrangian decomposition <i>Edrisi Muñoz, Elisabet Capón-García, Jose M. Laínez-Aguirre, Antonio Espuña, Luis Puigjaner</i>	989
An ontological approach to integration of planning and scheduling activities in the batch process industries <i>Marcela Vegetti, Gabriela Henning</i>	995
Constructing an ontology for physical-chemical processes <i>Heinz A. Preisig</i>	1001
Contributed Papers	
T-4: Process and Product Synthesis-Design	
Improved design strategies for flexible hydrogen networks <i>Chuei-Tin Chang, Che-Chi Kuo</i>	1007

An integrated reactive distillation process for biodiesel production <i>Eduardo S. Perez-Cisneros, Ricardo Morales-Rodriguez, Mauricio Sales-Cruz, Tomás Viveros-García, Ricardo Lobo-Oehmichen</i>	1013
A sequential algorithm for the rigorous design of thermally coupled distillation sequences <i>José A. Caballero, Juan A. Reyes-Labarta, Ignacio E. Grossmann</i>	1019
Discovery of new zeolites for H ₂ S removal through multi-scale systems engineering <i>Tingting Liu, Eric L. First, M. M. Faruque Hasan, Christodoulos A. Floudas</i>	1025
Optimization of a fusel oil separation system using a dividing wall column <i>José de Jesús Mendoza-Pedroza, Juan Gabriel Segovia-Hernández, Álvaro Orjuela-Londoño, Salvador Hernández</i>	1031
Silane production through reactive distillation with intermediate condensers <i>J. Rafael Alcántara-Avila, Hugo Alberto Sillas-Delgado, Juan Gabriel Segovia-Hernández, Fernando I. Gómez-Castro, Jorge A. Cervantes Jauregui</i>	1037
Optimal production of furfural and DMF from algae and switchgrass <i>Mariano Martín, Ignacio E. Grossmann</i>	1043
CO ₂ as feedstock: A new pathway to syngas <i>Flavio Manenti</i>	1049
Design and optimization of intensified non-sharp distillation configurations <i>Carlo E. Torres Ortega, Kasper Stricker, Massimiliano Errico, Ben-Guang Rong</i>	1055
Deterministic global optimization of multistage melt crystallization processes in hydroformylation <i>Christian Kunde, Achim Kienle</i>	1061
Design and economic evaluation of alternatives to effluents treatment on biodiesel production from soybean oil and palm oil <i>André F. Young, Fernando L. P. Pessoa, Eduardo M. Queiroz</i>	1067
Synthesis of transcritical ORC-integrated heat exchanger networks for waste heat recovery <i>Cheng-Liang Chen, Po-Yi Li, Hui-Chu Chen, Jui-Yuan Lee</i>	1073
Efficiency comparison of different design schemes of reactive distillation process for ethyl lactate production from fermentation-derived magnesium lactate <i>Boonpradab Dangpradab, Panarat Rattanaphanee</i>	1079
Tailor-made green diesel blends design using a decomposition-based computer-aided approach <i>Li Y. Phoon, Haslenda Hashim, Ramli Mat, Azizul A. Mustaffa</i>	1085
A mathematical programming targeting method to select treatment technologies ahead of design <i>Athanassios Lykourgos Nikolakopoulos, Antonis Kokossis</i>	1091
Optimal structure synthesis of ternary distillation system <i>Hiroshi Takase, Shinji Hasebe</i>	1097
Optimization and analysis of chemical synthesis routes for the production of biofuels <i>Douglas A. Allan, W. Alex Marvin, Srinivas Rangarajan, Prodromos Daoutidis</i>	1103
Design and economic evaluation of coal to synthetic natural gas (SNG) process <i>Bor-Yih Yu, I-Lung Chien</i>	1109
Water networks synthesis for industrial parks involving inter-plant allocation <i>Lin-lin Liu, Jian Wang, Jian-ping Li, Jian Du, Feng-lin Yang</i>	1115
Energy-saving design and control of a hybrid extraction/distillation system for the separation of pyridine and water <i>Yi-Chun Chen, I-Lung Chien</i>	1121

Alternative hybrid liquid-liquid and distillation sequences for the biobutanol separation <i>Massimiliano Errico, Eduardo Sanchez-Ramirez, Juan J. Quiroz-Ramirez, Juan G. Segovia-Hernández, Ben-Guang Rong</i>	1127
Integrated product and process design for the optimization of mayonnaise creaminess <i>Arend Dubbelboer, Jo Janssen, Ardjan Krijgsman, Edwin Zondervan, Jan Meuldijk</i>	1133
Synthesis of indirect work exchanger network based on transshipment model <i>Jian Du, Yu Zhuang, Lin-lin Liu, Ji-long Li, Jie Fan, Qing-wei Meng</i>	1139
Development of sustainable CO ₂ conversion processes for the methanol production <i>Kosan Roh, Tuan B. H. Nguyen, Uthaiporn Suriyapraphadilok, Jay H. Lee, Rafiqul Gani</i>	1145
Optimal design of algae biorefinery processing networks for the production of protein, ethanol and biodiesel <i>Peam Cheali, Anthony Vivion, Krist V. Gernaey, Gürkan Sin</i>	1151
Synthetic methane from CO ₂ : Dynamic optimization of the Sabatier process for power-to-gas applications <i>Ali El Sibai, Liisa Rihko-Struckmann, Kai Sundmacher</i>	1157
Inter-process heat integration by coordination among agent systems for heat exchanger network design <i>Naoki Kimura, Tetsuo Kaya, Shintaro Miyamoto, Yoshifumi Tsuge</i>	1163
Design and synthesis of batch processing plants: A consideration of utility aspect and using a robust scheduling platform <i>Esmael R. Seid, Thokozani Majazi</i>	1169
A novel approach for the identification of economic opportunities within the framework of a biorefinery <i>Ana I. Torres, Iwona Cybulska, Chuanji Fang, Mette H. Thomsen, Jens E. Schmidt, George Stephanopoulos</i>	1175
Integrated design and control of semicontinuous processes using mixed integer nonlinear dynamic optimization <i>Vida Meidanshahi, Thomas A. Adams II</i>	1181
A computational platform for simulation, design and analysis of a poly(lactic) acid production process from different lignocellulosic raw materials <i>Eduardo S. Pérez-Cisneros, Lourdes Avilés-Cabrera, Verónica Medina-Bañuelos, Mauricio Sales-Cruz, Alberto Ochoa-Tapia, Tomás Viveros-García, Ricardo Lobo-Ohemichen</i>	1187
Simultaneous design of desalination plants and distribution water network <i>Sebastián Herrera, Luis A. Cisternas, Edelmira D. Gálvez</i>	1193
Optimal design of microfluidic platforms for diffusion-based pcr for “one-pot” analysis of cells <i>Jordan Crow, Luke E. K. Achenie, Chang Lu, Sai Ma, Despina N. Loufakis, Zhenning Cao, Yiwen Chang</i>	1199
A systematic methodology for optimal mixture design in an integrated biorefinery <i>Lik Y. Ng, Viknesh Adniappan, Nishanth G. Chemmangattuvalappil, Denny K. S. Ng</i>	1205
A systematic visual approach to ionic liquid design for carbon dioxide capture <i>Fah K. Chong, Nishanth G. Chemmangattuvalappil, Dominic C. Y. Foo, Mert Atilhan, Fadwa T. Eljack</i>	1211
Intensification of C ₅ separation process by heat integration and thermal coupling <i>Hsiao-Ching Hsu, San-Jang Wang, John D.-Y. Ou, David S. H. Wong</i>	1217
Conceptual design of post-combustion CO ₂ capture processes - packed columns and membrane technologies <i>Mathias Leimbrink, Anna-Katharina Kunze, David Hellmann, Andrzej Górak, Mirko Skiborowski</i>	1223

Natural gas to liquid transportation fuels and olefins (GTL+C2_C4) <i>Onur Onel, Alexander M. Niziolek, Christodoulos A. Floudas</i>	1229
Life-cycle assessment principles for the integrated product and process design of polymers from CO ₂ <i>Niklas von der Assen, Mathias Lampe, Leonard Müller, André Bardow</i>	1235
Optimization-based methodology for wastewater treatment plant synthesis - a full scale retrofitting case study <i>Hande Bozkurt, Krist V. Gernaey, Gürkan Sin</i>	1241
An integrated framework for controllability assessment and solvent selection in post-combustion CO ₂ capture processes <i>Theodoros Damartzis, Athanasios I. Papadopoulos, Panos Seferlis</i>	1247
Using product driven process synthesis in the bio-refinery <i>Alexandra Kiskini, Edwin Zondervan, Peter Wierenga, Edwin Poiesz, Harry Gruppen</i>	1253
Integrating expanders into sub-ambient heat exchanger networks <i>Chao Fu, Truls Gundersen</i>	1259
Water free XTL processes: is it possible and at what cost? <i>Xinying Liu, Bilal Patel, Diane Hildebrandt</i>	1265
Energy and yield evaluation of an alcohols and hydrocarbons production plant using Rh-based catalysts with different promoters <i>Júlio C. C. Miranda, Gustavo H. S. F. Ponce, Harvey Arellano-Garcia, Rubens Maciel Filho, Maria R. Wolf Maciel</i>	1271
Computer-aided process analysis of an integrated biodiesel processes incorporating reactive distillation and organic solvent nanofiltration <i>Kathrin Werth, Kolja Neumann, Mirko Skiborowski</i>	1277
A thermodynamic targeting approach for the synthesis of sustainable biorefineries <i>Bilal Patel</i>	1283
A sustainability driven methodology for process synthesis in agro-food industry <i>Jochem Jonkman, Jacqueline M. Bloemhof, Jack G. A. J. van der Vorst, Albert van der Padt</i>	1289
Evaluation of dimethyl carbonate and ethylene glycol production from biomass <i>Chayanit Choomwattana, Aksornchan Chaianong, Worapon Kiatkittipong, Pichayapan Kongpanna, Suttichai Assabumrungrat</i>	1295
Simulation of carbon-dioxide-capture process using aqueous ammonia <i>Akrawin Jongpitisub, Kitipat Siemanond, Amr Henni</i>	1301
Energy efficient bioethanol purification by heat pump assisted extractive distillation in a dividing-wall column <i>Anton A. Kiss, Hao Luo, Costin S. Bildea</i>	1307
Process design of a multi-product lignocellulosic biorefinery <i>Aristide Giuliano, Massimo Poletto, Diego Barletta</i>	1313
MINLP optimization model for water/wastewater networks with multiple contaminants. <i>Kittichai Pungthong, Kitipat Siemanond</i>	1319
Design of separation processes with ionic liquids <i>Worawit Peng-noo, Kusuma Kulajapeng, Rafiqul Gani, Uthaiporn Suriyapraphadilok</i>	1325
Systematic screening of fermentation products as future platform chemicals for biofuels <i>Kristen Ulonska, Birgitta E. Ebert, Lars M. Blank, Alexander Mitsos, Jörn Viell</i>	1331
From fed-batch to continuous enzymatic biodiesel production <i>Jason Price, Matthias Nordblad, John M. Woodley, Jakob K. Huusom</i>	1337

Feed flexibility of CH ₄ combined reforming for methanol production <i>Benjamín Cañete, Nélide B. Brignole, Carlos E. Gigola</i>	1343
Process alternatives for second generation ethanol production from sugarcane bagasse <i>Felipe F. Furlan, Roberto C. Giordano, Caliane B. B. Costa, Argimiro R. Secchi, John M. Woodley</i>	1349
Simulation study of heat transfer enhancement due to wall boiling condition in a microchannel reactor block for Fischer-Tropsch synthesis <i>Krishnadas S. Kshetrimayum, Park Seongho, Jong Ikhwan, Na Jonggeol, Chonghun Han</i>	1355
CO ₂ vs biomass: Identification of environmentally beneficial processes for platform chemicals from renewable carbon sources <i>André Sternberg, Holger Teichgräber, Philip Voll, André Bardow</i>	1361
Design and optimization of intensified quaternary Petlyuk configuration <i>Massimiliano Errico, Pietro Pirellas, Ben-Guang Rong, Juan G. Segovia-Hernández</i>	1367
Techno-economic analysis of power and hydrogen co-production by an IGCC plant with CO ₂ capture based on membrane technology <i>Daniele Sofia, Aristide Giuliano, Massimo Poletto, Diego Barletta</i>	1373
Synthesis of water treatment processes using mixed integer programming <i>Mariya N. Koleva, Eleftheria M. Polykarpou, Songsong Liu, Craig A. Styan, Lazaros G. Papageorgiou</i>	1379
Viability of technologies for CO ₂ capture and reuse in a FPSO: Technical, economic and environmental analysis <i>Bruna C. S. Lima, Ofélia Q. F. Araújo, José L. de Medeiros, Cláudia R. V. Morgado</i>	1385
A superstructure-based framework for simultaneous process synthesis, heat integration, and utility plant design <i>S. Murat Sen, James A. Dumesic, Christos T. Maravelias</i>	1391
Process design and optimization of integrated shale gas process for green chemicals production <i>Chang He, Fengqi You</i>	1397
Value-added chemicals from microalgae: A sustainable process design using life cycle optimization <i>Jian Gong, Fengqi You</i>	1403
The effect of charge composition on the optimal operational parameters of a batch extractive distillation process <i>Laszlo Hegely, Peter Lang</i>	1409
VPPD Lab -The chemical product simulator <i>Sawitree Kalakul, Rehan Hussain, Nimir Elbashir, Rafiqul Gani</i>	1415
Synthesis of flexible heat exchanger networks integrated with reconfigurable control design <i>Lautaro Braccia, Patricio Luppi, Maximiliano García, Marta S. Basualdo</i>	1421
Computer-aided approach for designing solvents blend for herbal phytochemical extraction <i>Siti N. H. M. Azmin, Nor A. Yunus, Azizul A. Mustaffa, Sharifah R. W. Alwi, Lee S. Chua</i>	1427
Evolutionary algorithm for de novo molecular design considering multi-dimensional constraints <i>Robert H. Herring III, Mario R. Eden</i>	1433
Data mining and regression algorithms for the development of a QSPR model relating solvent structure and ibuprofen crystal morphology <i>Shounak Datta, Robert H. Herring III, Mario R. Eden</i>	1439
Designing reactants and products with properties dependent on both structures <i>Vikrant A. Dev, Nishanth G. Chemmangattuvalappil, Mario R. Eden</i>	1445

Conceptual design of an internally heat-integrated reactive distillation column based on thermodynamic and hydraulic analysis <i>Zixin Lin, Weizhong An, Yawei Xu, Jianmin Zhu</i>	1451
Carbon capture and utilisation: Application of life cycle thinking to process design <i>Rosa Cuellar-Franca, Ioanna Dimitriou, Pelayo Garcia-Gutierrez, Rachael H. Elder, Ray W. K. Allen, Adisa Azapagic</i>	1457
Topology optimization for biocatalytic microreactor configurations <i>Inês P. Rosinha, Krist V. Gernaey, John M. Woodley, Ulrich Krühne</i>	1463
Design of hybrid heat-integrated configuration for indirect reactive distillation processes <i>Kuo-Chun Weng, Hao-Yeh Lee</i>	1469
Optimization of ionic liquid recycling in Ionic Liquid-based Three Phase Partitioning processes <i>Enrique Alvarez-Guerra, Angel Irabien</i>	1475
Optimization of the Integrated Gasification Combined Cycle Using Advanced Mathematical Models <i>Bongani Mvelase, Thokozani Majozi</i>	1481
Contributed Papers	
T-5: Process Dynamics, Control and Monitoring	
Nonparametric soft sensor evaluation for industrial distillation plant <i>Andrey Torgashov, Konstantin Zmeu</i>	1487
Comparing temperature difference control schemes for dividing-wall distillation columns <i>Yang Yuan, Haisheng Chen, Jieping Yu, Kejin Huang</i>	1493
A decentralised multi-parametric model predictive control study for a domestic heat and power cogeneration system <i>Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos</i>	1499
A control strategy for periodic systems - application to the twin-column MCSGP <i>Maria M. Papathanasiou, Fabian Steinebach, Guido Stroehlein, Thomas Müller-Späth, Ioana Nascu, Richard Oberdieck, Massimo Morbidelli, Athanasios Mantalaris, Efstratios N. Pistikopoulos</i>	1505
Design of multiparametric NCO-tracking controllers for linear dynamic systems <i>Muxin Sun, Benoît Chachuat, Efstratios N. Pistikopoulos</i>	1511
A performance-oriented robust framework for the online model-based optimization and control of (fed-) batch systems <i>Francesco Rossi, Flavio Manenti, Gintaras V. Reklaitis, Guido Buzzi-Ferraris</i>	1517
Raman-based advanced control of an absorption desorption system <i>Erik Esche, David Müller, Michael Maiwald, Günter Wozny</i>	1523
A comparative study between neural networks (NN)-based and adaptive-PID controllers for the optimal bio-hydrogen gas production in microbial electrolysis cell reactor <i>Azwar M. Yahya, Mohd A. Hussain, A. K. Abdul Wahab, M. F. Zamil</i>	1529
Reaction monitoring of cementing materials through multivariate techniques applied to in situ synchrotron X-ray diffraction data <i>Alessandra Taris, Massimiliano Grosso, Mariarosa Brundu, Vincenzo Guida, Alberto Viani</i>	1535
Multivariate fault isolation using lasso-based penalized discriminant analysis <i>Te-Hui Kuang, Zhengbing Yan, Yuan Yao</i>	1541
Flexible operation of CO ₂ capture processes integrated with power plant using advanced control techniques <i>Ana-Maria Cormos, Mihaela Vasile, Mircea-Vasile Cristea</i>	1547

Modified minimum variance approach for state and unknown input estimation <i>Yukteshwar Baranwal, Pushkar Ballal, Mani Bhushan</i>	1553
A new software development methodology for controllability analysis of forced circulation evaporator system <i>Afshin Sadrieh, Parisa A. Bahri</i>	1559
A nonlinear quasi-unknown input observer for the chemostat droop model <i>Alexander Schaum, Thomas Meurer</i>	1565
PAT for reactive crystallization process optimization for phosphorus recovery from sewage sludge <i>Yi Liu, Haiyan Qu</i>	1571
Time-optimal operation of diafiltration processes in the presence of fouling <i>Martin Jelemenský, Ayush Sharma, Radoslav Paulen, Miroslav Fikar</i>	1577
Supercritical gas recycle analysis for surge control of centrifugal compressors <i>Sara Budinis, Nina F. Thornhill</i>	1583
Software sensors design and selection for the production of biodiesel from grease trap wastes <i>Efrén Aguilar-Garnica, Juan P. García-Sandoval</i>	1589
Improving data reliability for process monitoring with fuzzy outlier detection <i>Harakhun Tanatavikorn, Yoshiyuki Yamashita</i>	1595
Inversion-based feedforward control design for the droop model <i>Alexander Schaum, Thomas Meurer</i>	1601
Effect of solvent content on controllability of extractive distillation columns <i>Wagner B. Ramos, Marcella F. Figueirêdo, Karoline D. Brito, Romildo P. Brito</i>	1607
High purity, high recovery, multi-component methanol distillation control <i>Isuru A. Udugama, Tajammal Munir, Robert Kirkpatrick, Brent R. Young, Wei Yu</i>	1613
Implementation of model predictive control in industrial gasoline desulfurization process <i>Kornkrit Chiewchanchairat, Pornchai Bumroongsri, Veerayut Lersbamrungsuk, Amornchai Apornwichanop, Soorathep Kheawhom</i>	1619
Maximizing profit of semi batch autocatalytic esterification process in the presence of disturbance: application of cascaded-conditional based online dynamic optimization <i>Fakhrony S. Rohman, Suhairi A. Sata, Norashid Aziz</i>	1625
MIMO neural Wiener based model predictive control (NWMPC) for MTBE reactive distillation using simulated annealing- particle swarm optimization (SA-PSO) <i>Muhamad N. Murat, Sudibyo, Norashid Aziz</i>	1631
A real time particle size control framework in non-isothermal antisolvent crystallization processes <i>Navid Ghadipasha, Stefania Tronci, Roberto Baratti, Jose A. Romagnoli</i>	1637
Multivariable adaptive Lyapunov fuzzy controller for pH neutralisation process <i>Mohd F. Zani, Mohd A. Hussain</i>	1643
Detection of changes in fouling behaviour by simultaneous monitoring of thermal and hydraulic performance of refinery heat exchangers <i>Emilio Díaz-Bejarano, Francesco Coletti, Sandro Macchietto</i>	1649
Dosage of filter aids in the case of pure surface filtration – an optimal control approach <i>Michael Kuhn, Heiko Briesen</i>	1655
Best of breed control of platinum precipitation reactors <i>Rotimi Agbebi, Carl Sandrock</i>	1661
Multivariate analysis of industrial scale fermentation data <i>Lisa Mears, Rasmus Nørregård, Stuart M. Stocks, Mads O. Albaek, Gürkan Sin, Krist V. Gernaey, Kris Villez</i>	1667

Model-based observation and design of crystal shapes via controlled growth-dissolution cycles <i>Holger Eisenschmidt, Naim Bajcinca, Kai Sundmacher</i>	1673
Adsorption based competitive purity control in crystallization <i>Akos Borsos, Zoltan K. Nagy</i>	1679
Stabilizing control for reactor/separator processes with gas and liquid recycles <i>Hiroya Seki</i>	1685
Extended VRFT method for controller design of nonlinear systems based on block-oriented model structures <i>Jyh-Cheng Jeng, Yi-Wei Lin, Min-Wei Lee</i>	1691
Linear or nonlinear? Comparing measures of nonlinearity <i>Malik M. Tahiyat, M. A. A. Shoukat Choudhury</i>	1697
Model predictive control for the self-optimized operation in wastewater treatment plants <i>Mario Francisco, Sigurd Skogestad, Pastora Vega</i>	1703
Off-line tube-based robust model predictive control for uncertain and highly exothermic polymerization processes <i>Pornchai Bumroongsri, Veerayut Lersbamrungsuk, Soorathep Kheawhom</i>	1709
Optimization based constrained unscented gaussian sum filter <i>Krishna K. Kottakki, Sharad Bhartiya, Mani Bhushan</i>	1715
Systematic control structure evaluation of two-stage-riser fluidized catalytic pyrolysis processes <i>Zhihong Yuan, Ping Wang, Mario R. Eden</i>	1721
Novel data segmentation methods for data driven process analyses <i>Rajesh Paul, M. A. A. Shoukat Choudhury</i>	1727
Robust model predictive control strategy for LTV and LPV systems of the internal reforming solid oxide fuel cell <i>Narissara Chatrattanawet, Soorathep Kheawhom, Amornchai Arpornwichanop</i>	1733
Plantwide predictive monitoring of sulfur emissions in tail gas treatment units <i>Eva M. Speelmanns, Francesco Rossi, Andres R. Leon-Garzon, Flavio Manenti</i>	1739
Robust control of industrial propylene-propane fractionation process <i>Cristian Patrascioiu, Nicolae Paraschiv, Anh C. Minh, Marian Popescu</i>	1745
Improved optimization-based design of PID controllers using exact gradients <i>Chriss Grimholt, Sigurd Skogestad</i>	1751
Enhancing xylitol bio-production by an optimal feeding policy during fed-batch operation <i>Oscar A. Prado-Rubio, Héctor Hernández-Escoto, Divanery Rodriguez-Gomez, Sarote Sirisansaneeyakul, Ricardo Morales-Rodriguez</i>	1757
Performance evaluation of bayesian state estimators for nonlinear dae systems using a moderately high dimensional reactive distillation column model <i>Jalesh L. Purohit, Sachin C. Patwardhan, Sanjay M. Mahajani</i>	1763
State estimation in fermentation of lignocellulosic ethanol. Focus on the use of pH measurements <i>Miguel Mauricio-Iglesias, Krist V. Gernaey, Jakob K. Huusom</i>	1769
Dynamic simulation and analysis of slug flow impact on offshore natural gas processing: TEG dehydration, Joule-Thomson expansion and membrane separation <i>Lara de O. Arinelli, Ofélia Q. F. Araújo, José L. de Medeiros</i>	1775
Contributed Papers	
T-6: Abnormal Events Management and Process Safety	
Automata based test plans for fault diagnosis in batch processes <i>Chuei-Tin Chang, Wei-Chung Hsieh</i>	1781

Modelling and monitoring of natural gas pipelines: new method for leak detection and localization estimation <i>Xinghua Pan, M. Nazmul Karim</i>	1787
Dynamic artificial immune system with variable selection based on causal inference <i>Yidan Shu, Jinsong Zhao</i>	1793
A smart safety system for chemical processes <i>Rafael M. Soares, Argimiro R. Secchi, José C. Pinto</i>	1799
Shape constrained splines with discontinuities for anomaly detection in a batch process <i>Kris Villez, Jonathan Habermacher</i>	1805
Quantifying model uncertainty in scarce data regions – a case study of particle erosion in pipelines <i>Wei Dai, Selen Cremaschi</i>	1811
Leak identification using extended Kitanidis-Kalman filter <i>C. Ganesh, Pushkar Ballal, Mani Bhushan, Sachin C. Patwardhan</i>	1817
Process monitoring and fault detection in non-linear chemical process based on multi-scale kernel Fisher discriminant analysis <i>Norazwan M. Nor, Mohd A. Hussain, Che R. C. Hassan</i>	1823
Hierarchical fault propagation and control strategy from the resilience engineering perspective: A case study with petroleum refining system <i>Jinqiu Hu, Laibin Zhang, Xi Ma, Zhansheng Cai</i>	1829
Risk analysis applied to bioethanol dehydration processes: azeotropic distillation versus extractive distillation <i>Adriana Avilés-Martínez, Nancy Medina-Herrera, Arturo Jiménez-Gutiérrez, Medardo Serna-González, Agustín J. Castro-Montoya</i>	1835
Contributed Papers	
T-7: Plant Operations, Integration, Planning /Scheduling and Supply Chain	
Supply chain design and planning accounting for the triple bottom line <i>Bruna A. Mota, Maria Isabel Gomes, Ana Carvalho, Ana P. Barbosa-Póvoa</i>	1841
Planning of a multiproduct pipeline integrating blending and distribution <i>Diovanina Dimas, Valéria V. Murata, Sérgio M. S. Neiro, Susana Relvas, Ana P. Barbosa-Póvoa</i>	1847
Optimal multi-period investment analysis for flexible pulp mill utility systems <i>Elin Svensson</i>	1853
Scenario-based price negotiations vs. game theory in the optimization of coordinated supply chains <i>Kefah Hjaila, Luis Puigjaner, Antonio Espuña</i>	1859
On the complexity of production planning and scheduling in the pharmaceutical industry: the Delivery Trade-offs Matrix <i>Samuel Moniz, Ana P. Barbosa-Póvoa, Jorge Pinho de Sousa</i>	1865
Flare minimization of ethylene plant start-up via resource-task network approach <i>Guang Song, Tong Qiu, Bingzhen Chen</i>	1871
Phenomenological decomposition heuristic for process design synthesis of oil-refinery units <i>Brenno C. Menezes, Jeffrey D. Kelly, Ignacio E. Grossmann</i>	1877
A value chain optimisation model for a biorefinery with feedstock and product choices <i>Madeleine J. Bussemaker, Kenneth Day, Geoffrey Drage, Franjo Cecelja</i>	1883
Downstream petroleum supply chains planning under uncertainty <i>Leão J. Fernandes, Susana Relvas, Ana P. Barbosa-Póvoa</i>	1889
Optimal management of shuttle robots in a laboratory automation system of a cement plant <i>Christian Schoppmeyer, Christian Sonntag, Siddharth Gajjala, Sebastian Engell</i>	1895

A novel approach to predict violations and to define the reference contaminant and operation in water using networks <i>Ewerton E. S. Calixto, Flávio S. Francisco, Fernando L. P. Pessoa, Eduardo M. Queiroz</i>	1901
MDP formulation and solution algorithms for inventory management with multiple suppliers and supply and demand uncertainty <i>Joohyun Shin, Jay H. Lee</i>	1907
Optimal design of closed-loop supply chain networks with multifunctional nodes <i>Magdalini A. Kalaitzidou, Pantelis Longinidis, Michael C. Georgiadis</i>	1913
Simultaneous optimisation of economic and environmental objectives with dynamic price signals and operational constraints <i>Tristan Lambert, Andrew F. A. Hoadley, Barry Hooper</i>	1919
Integration of scheduling and vessel routing in pipeless plants <i>Munawar A. Shaik, Pulkit Mathur</i>	1925
A mean value cross decomposition strategy for demand-side management of a pulping process <i>Hubert Hadera, Per Wide, Iiro Harjunoski, Juha Mäntysaari, Joakim Ekström, Guido Sand, Sebastian Engell</i>	1931
Tighter integration of maintenance and production in short-term scheduling of multipurpose process plants <i>Matteo Biondi, Guido Sand, Iiro Harjunoski</i>	1937
Integrating control and scheduling based on real-time detection of divergence <i>Preeti Rathi, Shanmukha M. Bhumirreddy, Naresh N. Nandola, Iiro Harjunoski, Rajagopalan Srinivasan</i>	1943
Resource efficiency indicators for real-time monitoring and optimization of integrated chemical production plants <i>Marc Kalliski, Daniel Krahe, Benedikt Beisheim, Stefan Krämer, Sebastian Engell</i>	1949
A meta-multiparametric framework: Application to the operation of bio-based energy supply chains <i>Sergio Medina, Ahmed Shokry, Javier Silvente, Antonio Espuña</i>	1955
A continuous-time MILP model for direct heat integration in batch plants <i>Pedro M. Castro, Bruno Custódio, Henrique A. Matos</i>	1961
Improving pharmaceutical batch production processes with data-based tiered approach <i>Lukas G. Eberle, Hirokazu Sugiyama, Stavros Papadokonstantakis, Andreas Graser, Rainer Schmidt, Konrad Hungerbühler</i>	1967
Integrated cyclic scheduling and operation optimization for cracking furnaces system considering feed changeover <i>Yangkun Jin, Jinlong Li, Wenli Du, Feng Qian</i>	1973
MINLP model and two-level algorithm for the simultaneous synthesis of heat exchanger networks and utility systems <i>Emanuele Martelli, Alberto Mian, François Maréchal</i>	1979
Process simulations supporting a techno-economic framework to optimize the biorefinery supply chains <i>Sumesh Sukumara, Kwabena Darkwah, Jeffrey R. Seay</i>	1985
A rescheduling algorithm for a large-scale reverse osmosis desalination plant under uncertain fresh water demand <i>Jian Wang, Aipeng Jiang, Lekai Lian, Guohui Huang, Qiang Ding, Shu Jiangzhou</i>	1991

Water exchange in eco-industrial parks through multiobjective optimization and game theory <i>Manuel Ramos, Marianne Boix, Didier Aussel, Ludovic Montastruc, Patrick Vilamajo, Serge Domenech</i>	1997
Conceptual design of cost-effective and environmentally-friendly configurations for an integrated industrial complex <i>Chen Chen, Ross Wakelin</i>	2003
Modelling of environmental impacts and economic benefits of fiber reinforced polymers composite recycling pathways <i>Phuong A. Vo Dong, Catherine Azzaro-Pantel, Marianne Boix, Leslie Jacquemin, Serge Domenech</i>	2009
A MILP transshipment model to integrate and re-engineer distillation columns into overall processes. <i>Konstantinos A. Pyrgakis, Kipouros P. Ioannis, Antonis C. Kokossis</i>	2015
A duality-based approach for bilevel optimization of capacity expansion <i>Pablo Garcia-Herreros, Pratik Misra, Erdem Arslam, Sanjay Mehta, Ignacio E. Grossmann</i>	2021
A hybrid CP/MILP approach for big size scheduling problems of multiproduct, multistage batch plants <i>Franco M. Novara, Gabriela P. Henning</i>	2027
Optimal scheduling of liquid drug product manufacturing <i>Lukas G. Eberle, Elisabet Capón-Garcia, Martin Senninger, Hirokazu Sugiyama, Andreas Graser, Rainer Schmidt, Konrad Hungerbühler</i>	2033
Optimization of petrochemical process planning using naphtha price forecast and process modeling <i>Hweeung Kwon, Byeonggil Lyu, Kyungjae Tak, Jinsuk Lee, Il Moon</i>	2039
Contributed Papers	
T-8: Enterprise-wide Management and Technology-driven Policy Making	
Agent-based model of the German biodiesel supply chain <i>Jorge A. Moncada, Martin Junginger, Zofia Lukszo, André Faaij, Margot Weijnen</i>	2045
A study of the sustainable development of China's phosphorus resources industry based on system dynamics <i>Shujie Ma, Shanying Hu, Dingjiang Chen, Yuzhong Feng</i>	2051
Interplant carbon integration towards phased footprint reduction targets <i>Dhabia M. Al-Mohannadi, Patrick Linke, Sumit K. Bishnu, Sabla Y. Almouri</i>	2057
Decision support by multicriteria optimization in process development: An integrated approach for robust planning and design of plant experiments <i>Michael Bortz, Volker Maag, Jan Schwientek, Regina Benfer, Roger Böttcher, Jakob Burger, Erik von Harbou, Norbert Asprion, Karl-Heinz Küfer, Hans Hasse</i>	2063
Product and process network modelling and pathway optimization with life cycle functional analysis: the case of biofuels <i>Daniel Garcia, Fengqi You</i>	2069
Contributed Papers	
T-9.1: Molecular Systems Engineering	
Computer-aided design of solvents for the recovery of a homogeneous catalyst used for alkene hydroformylation <i>Kevin McBride, Kai Sundmacher</i>	2075
Computational molecular design of a water-compatible dentin adhesive system <i>Farhana Abedin, Brock Roughton, Paulette Spencer, Qiang Ye, Kyle V. Camarda</i>	2081

An evaluation of thermodynamic models for the prediction of solubility of phytochemicals from orthosiphon staminues in ethanol 2087
Mohd S. M. Nor, Zainuddin A. Manan, Azizul A. Mustaffa, Chua L. Suan

Computer-aided framework for design of pure, mixed and blended products 2093
Stefano Cignitti, Lei Zhang, Rafiqul Gani

Contributed Papers

T-9.2: Biological Systems Engineering

Uncertainty in clinical data and stochastic model for in-vitro fertilization 2099
Kirti M. Yenkie, Urmila M. Diwekar

Mathematical analysis of multistage population balances for cell growth and death 2105
Margaritis Kostoglou, María Fuentes-Garí, David García-Münzer, Michael C. Georgiadis, Nicki Panoskaltsis, Efstratios N. Pistikopoulos, Athanasios Mantalaris

Oxygen transfer rates and requirements in oxidative biocatalysis 2111
Asbjørn Toftgaard Pedersen, Gustav Rehn, John M. Woodley

Robust process design for the bioproduction of b-carotene in green microalgae 2117
Robert J. Flassig, Melanie Fachet, Liisa Rihko-Struckmann, Kai Sundmacher

Exploring opportunities for the production of chemicals from municipal solid wastes within the framework of a biorefinery 2123
Fabian Bonk, Tanmay Chaturvedi, Ana I. Torres, Jens E. Schmidt, Mette H. Thomsen, George Stephanopoulos

Development of a macroscopic model for the production of bioethanol with high yield and productivity via the fermentation of phalaris aquatica l. Hydrolysate 2129
Anna Karapatsia, Giannis Penloglou, Christos Chatzidoukas, Costas Kiparissides

Enzymatic reactive distillation for the transesterification of ethyl butyrate: model validation and process analysis 2135
Matthias Wierschem, Rene Heils, Stefan Schlimper, Irina Smirnova, Andrzej Górak, Philip Lutze

Design of a gene metabolator under uncertainty 2141
Asif H. Bhatti, Geraint Thomas, Vivek Dua

Manufacturability indices for high-concentration monoclonal antibody formulations 2147
Yang Yang, Ajoy Velayudhan, Nina F. Thornhill, Suzanne S. Farid

Experimental validation of in silico flux predictions from a genome-scale model (iMM518) for carbon dioxide utilization by *M. maripaludis* 2153
Nishu Goyal, Iftekhar A. Karimi, Zhi Zhou

Contributed Papers

T-9.3: Pharmaceutical Systems Engineering

Cell cycle model selection for leukemia and its impact in chemotherapy outcomes 2159
María Fuentes-Garí, Ruth Misener, Eleni Pefani, David García-Münzer, Margaritis Kostoglou, Michael C. Georgiadis, Nicki Panoskaltsis, Efstratios N. Pistikopoulos, Mantalaris Athanasios

Model-based characterisation of twin-screw granulation system for continuous solid dosage manufacturing 2165
Ashish Kumar, Krist V. Gernaey, Thomas De Beer, Ingmar Nopens

Process-based method for reducing product losses in pharmaceutical manufacturing 2171
Hirokazu Sugiyama, Masaaki Ito, Masahiko Hirao

Model-based optimization of the primary drying step during freeze-drying 2177
Séverine T.F.C. Mortier, Pieter-Jan Van Bockstal, Ingmar Nopens, Krist V. Gernaey, Thomas De Beer

Plant-wide control of a continuous tablet manufacturing for Quality-by-Design based pharmaceutical manufacturing <i>Ravendra Singh, Fernando Muzzio, Marianthi Ierapetritou, Rohit Ramachandran</i>	2183
Systematic retrofitting methodology for recrystallization of thermally unstable active pharmaceutical ingredients <i>Gioele Casola, Hirokazu Sugiyama, Satoshi Yoshikawa, Hayao Nakanishi, Masahiko Hirao</i>	2189
Modeling of crystallization of solid oral drug forms in a dropwise additive manufacturing system <i>Elçin İçten, Zoltan K. Nagy, Gintaras V. Reklaitis</i>	2195
Macroporous microparticles for pharmaceutical and medical applications <i>Alexandra Zhukova, Alexander Troyankin, Aleksandr Didenko, Natalia Menshutina</i>	2201
Optimal resin selection for integrated chromatographic separations in high-throughput screening <i>Songsong Liu, Spyridon Gerontas, David Gruber, Richard Turner, Nigel J. Titchener-Hooker, Lazaros G. Papageorgiou</i>	2207
Plantwide design and economic evaluation of two Continuous Pharmaceutical Manufacturing (CPM) cases: Ibuprofen and Artemisinin <i>Hikaru G. Jolliffe, Dimitrios I. Gerogiorgis</i>	2213
Contributed Papers	
T-9.4: Food Systems Engineering	
Data-based multivariate modeling of a grain comminution process <i>Filippo Dal-Pastro, Pierantonio Facco, Fabrizio Bezzo, Helen Thomas, Eliana Zamprogna, Massimiliano Barolo</i>	2219
A comprehensive sensitivity and uncertainty analysis of a milk drying process <i>Adrián Ferrari, Soledad Gutiérrez, Gürkan Sin</i>	2225
Optimization of production planning and scheduling in the ice cream industry <i>Mariana C. R. Carvalho, Tânia Pinto-Varela, Ana P. Barbosa-Póvoa, Pedro Amorim, Bernardo Almada-Lobo</i>	2231
Contributed Papers	
T-9.5: Energy Systems Engineering	
Evaluation of energy integration aspects for advanced chemical looping systems applied for energy vectors poly-generation <i>Calin-Crisitan Cormos, Ana-Maria Cormos, Paul-Serban Agachi</i>	2237
Synthesis of biomass-based trigeneration systems with reliability aspects <i>Viknesh Andiappan, Raymond R. Tan, Kathleen B. Aviso, Denny K. S. Ng</i>	2243
Optimization of the cost of compression in the Finnish natural gas pipeline <i>Markéta Mikolajková, Henrik Saxén, Frank Pettersson</i>	2249
An approach to optimize multi-enterprise biofuel supply chains including Nash equilibrium models <i>Ricardo A. Ortiz-Gutiérrez, Sara Giarola, Nilay Shah, Fabrizio Bezzo</i>	2255
Optimal integration of the year-round operation for methane production from CO ₂ and water using wind, solar and biomass <i>Mariano Martín, William Davis</i>	2261
Optimal scheduling of air separation with cryogenic energy storage <i>Qi Zhang, Clara F. Heuberger, Ignacio E. Grossmann, Arul Sundaramoorthy, Jose M. Pinto</i>	2267
An integrated unit commitment and generation expansion planning model <i>Nikolaos E. Koltsaklis, Michael C. Georgiadis</i>	2273

System design of renewable energy generation and storage alternatives for large scale continuous processes	2279
<i>Oluwamayowa Amusat, Paul Shearing, Eric S. Fraga</i>	
Energy assessment of different configurations for the ethanol production process from lignocellulosic biomass	2285
<i>Cristian F. Triana, Eric S. Fraga, Eva Sorensen</i>	
Integrated solar thermal hydrogen and power coproduction process for continuous power supply and production of chemicals	2291
<i>Emre Gençer, Mohit Tawarmalani, Rakesh Agrawal</i>	
Energy supply chain modeling for the optimisation of a large scale energy planning problem	2297
<i>Christiana Papapostolou, Emilia Kondili, Ioannis K. Kaldellis, Wolf G. Früh</i>	
Synthesis of optimal processing pathway for microalgae-based biorefinery under uncertainty	2303
<i>Muhammad Rizwan, Jay H. Lee, Rafiqul Gani</i>	
Effect of feed natural gas conditions on the performance of mixed refrigerant LNG process	2309
<i>Mengyu Wang, Rajab Khalilpour, Ali Abbas</i>	
A spatial decomposition procedure for effective solution of two dimensional energy distribution problems	2315
<i>Carl Haikarainen, Frank Pettersson, Henrik Saxén</i>	
A rolling horizon stochastic programming framework for the energy supply and demand management in microgrids	2321
<i>Javier Silvente, Georgios M. Kopanos, Antonio Espuña</i>	
Behaviour assessment of a fuel cell - battery system using a supervisory control methodology empowered by a hybrid timed automaton (HTA)	2327
<i>Chrysovalantou Ziogou, Damian Giaouris, Christos Yfoulis, Fotis Stergiopoulos, Spyros Voutetakis, Simira Papadopoulou</i>	
Financial considerations in shale gas supply chain development	2333
<i>Andrés J. Calderón, Omar J. Guerra, Lazaros G. Papageorgiou, Jeffrey J. Sirola, Gintaras V. Reklaitis</i>	
Optimal dynamic operation of adsorption-based energy systems driven by fluctuating renewable energy	2339
<i>Uwe Bau, Anna-Lena Braatz, Franz Lanzerath, Michael Herty, André Bardow</i>	
A spatial multi-period mixed integer linear programming (MILP) model for optimal power planning: CO2 emissions mitigation	2345
<i>Omar J. Guerra, Diego A. Tejada, Raúl Rodríguez, Gintaras V. Reklaitis</i>	
Bringing non-energy systems into bioenergy value chain optimization framework	2351
<i>Miao Guo, Nilay Shah</i>	
MILP approach for the design of residential microgrids with energy interaction restrictions	2357
<i>Carmen Wouters, Eric S. Fraga, Adrian M. James</i>	
Engineering design of localised synergistic production systems	2363
<i>Melissa Y. Leung Pah Hang, Elias Martinez-Hernandez, Matthew Leach, Aidong Yang</i>	
Modeling multi stream heat exchangers using operational data	2369
<i>Harsha N. Rao, Iftekhar A. Karimi</i>	
Improving the energy efficiency of cryogenic air separation units (ASU) through compressor waste heat recovery using direct binary heat engine cycle	2375
<i>Mathew Aneke, Meihong Wang</i>	
IGCC modeling for simultaneous power generation and CO2 capture	2381
<i>Usama Ahmed, Umer Zahid, Chonghun Han</i>	

Structural similarities and differences between smart grids and process industry supply chains: India case study	2387
<i>Nikita Patel, Rishabh Abhinav, Babji Srinivasan, Rajagopalan Srinivasan</i>	
Integrated computational and experimental studies of microalgal production of fuels and chemicals	2393
<i>Mesut Bekirogullari, Jon Pittman, Constantinos Theodoropoulos</i>	
Process integration and assessment of biogas systems	2399
<i>Bin Wu, Yajing Xu, Xiangping Zhang</i>	
Development and parameter estimation for an enhanced multivariate Herschel-Bulkley rheological model of a nanoparticle-based smart drilling fluid	2405
<i>Dimitrios I. Gerogiorgis, Christina Clark, Zisis Vryzas, Vassilios C. Kelessidis</i>	
Adaptive management of renewable energy smart grids using a power grand composite curves approach	2411
<i>Damian Giaouris, Athanasios I. Papadopoulos, Panos Seferlis, Simira Papadopoulou, Spyros Voutetakis</i>	
Impact of the operating conditions and position of exhaust gas recirculation on the performance of a micro gas turbine	2417
<i>Usman Ali, Carolina F. Palma, Kevin J. Hughes, Derek B. Ingham, Lin Ma, Mohamed Pourkashanian</i>	
Dynamic response of fuel cell gas turbine hybrid to fuel composition changes using hardware-based simulations	2423
<i>Nor F. Harun, David Tucker, Thomas A. Adams II</i>	
Short-term planning of cogeneration power plants: a comparison between MINLP and piecewise-linear MILP formulations	2429
<i>Leonardo Taccari, Edoardo Amaldi, Emanuele Martelli, Aldo Bischi</i>	
Optimum facility location and plant scheduling for biofuel production	2435
<i>Chen Li, Selen Cremaschi</i>	
Energy consumption scheduling of smart homes with microgrid under multi-objective optimisation	2441
<i>Di Zhang, Sara Evangelisti, Paola Lettieri, Lazaros G. Papageorgiou</i>	
Optimization of pressure/vacuum swing adsorption with variable dehydration levels and material selection for post combustion carbon capture	2447
<i>Karson T. Leperi, Randall Q. Snurr, Fengqi You</i>	
A drilling scheduling toolbox for oil and gas reservoirs	2453
<i>M. S. Tavallali, F. Bakhtazma, A. Meymandpour, F. Sadeghi, M. Hamed, I. A. Karimi</i>	
Preliminary analysis of systems for integrating solar thermal energy into processes with heat demands	2459
<i>Andreja Nemet, Jiří J. Klemeš, Zdravko Kravanja</i>	
Contributed Papers	
T-9.6: Environmental Systems Engineering	
Process simulation of ammonia recovery from biogas digestate by air stripping with reduced chemical consumption.	2465
<i>Lene F. Sjøtoft, Michael B. Pryds, Anne K. Nielsen, Birgir Norddahl</i>	
WWSO for distributed treatment of effluents	2471
<i>Lorena P. M. Moreira, Bernadete E. P. C. Delgado, Eduardo M. Queiroz, Fernando L. P. Pessoa</i>	
Extending the benchmark simulation model NO2 with processes for nitrous oxide production and side-stream nitrogen removal	2477
<i>Riccardo Boiocchi, Krist V. Gernaey, Gürkan Sin</i>	

A framework for the dynamic modelling of PI curves in microalgae <i>Andrea Bernardi, Andreas Nikolaou, Andrea Meneghesso, Benoît Chachuat, Tomas Morosinotto, Fabrizio Bezzo</i>	2483
Progresses of PSE studies on water networks and industrial application practices in China <i>Youqi Yang, Xiaoping Jia, Lei Shi, Qinxian Zhuang</i>	2489
Multi-objective optimization of small-size wastewater treatment plants operation <i>Rainier Hreiz, Nicolas Roche, Brahim Benyahia, M. Abderrazak Latifi</i>	2495
Pipeline merging considerations for the synthesis and design of interplant water networks with wastewater treatment, regeneration and reuse <i>Sabla Y. Alnouri, Patrick Linke, Mahmoud El-Halwagi</i>	2501
Simultaneous design and planning of CO ₂ transport pipeline network for carbon dioxide capture and sequestration project <i>Xiong Zou, Hongguang Dong, Jian Li, Jingqu Wang</i>	2507
Environmental, societal and economical optimization of a bioethanol supply chain <i>Carlos Miret, Ludovic Montastruc, Stéphane Negny, Serge Domenech</i>	2513
Operation optimization of ammonia-nitrogen removal process in coking wastewater treatment <i>Yuehong Zhao, Mingsen Liao, Pengge Ning, Hongbin Cao, Hao Wen</i>	2519
Solubility measurement and process simulation of CO ₂ /CH ₄ gas mixtures using ionic liquids <i>Jubao Gao, Yajing Xu, Xin Zhang, Xiangping Zhang</i>	2525
Evaluation of qualitative trend analysis as a tool for automation <i>Christian M. Thürlimann, David J. Dürrenmatt, Kris Villez</i>	2531
A detailed mathematical modelling representation of clean water treatment plants <i>Folashade Akinmolayan, Nina F. Thornhill, Eva Sorensen</i>	2537
Water resources management with dynamic optimization strategies and integrated models of lakes and artificial wetlands <i>Jimena Di Maggio, Vanina Estrada, M. Soledad Diaz</i>	2543
Life cycle assessment studies of chemical and biochemical processes through the new LCSof software-tool <i>Perapong Supawanich, Pomthong Malakul, Rafiqul Gani</i>	2549
Control structure design of an innovative enhanced biological nutrient recovery activated sludge system coupled with a photobioreactor <i>Borja Valverde-Pérez, José M. Fuentes-Martínez, Xavier Flores-Alsina, Krist V. Gernaey, Jakob K. Huusom, Benedek Gy. Plósz</i>	2555
Contributed Papers	
Renenseng EU-Project	
Production of phthalic anhydride from biorenewables: process design <i>Sara Giarola, Charles Romain, Charlotte K. Williams, Jason P. Hallett, Nilay Shah</i>	2561
Model integration using ontology input-output matching <i>Linsey Koo, Franjo Cecelja</i>	2567
Life cycle assessment of biorefinery products based on different allocation approaches <i>Paraskevi Karka, Stavros Papadokonstantakis, Konrad Hungerbühler, Antonis Kokossis</i>	2573
Sustainable process design under uncertainty analysis: targeting environmental indicators <i>Carina L. Gargalo, Gürkan Sin</i>	2579
Optimization of LNG Plant Operating Conditions to Anticipate Leaner Feed Gas by Steady State Process Simulation <i>Ferry Adhi Perdana, Johan Anindito Indriawan</i>	2585