

Computing and Systems Technology Division

Presentations at the 2010 AIChE Annual Meeting

**Salt Lake City, Utah, USA
7-12 November 2010**

Volume 1 of 2

ISBN: 978-1-61782-156-1

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2010) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2011)

For permission requests, please contact AIChE
at the address below.

AIChE
3 Park Avenue
New York, NY 10016-5991

Phone: (203) 702-7660
Fax: (203) 775-5177

www.aiche.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

Volume 1

Design of Massive Energy Storage Systems for IGCC Based Electric Power Generation	1
<i>Donald J. Chmielewski, Ming-Wei Yang</i>	
A Decomposition Algorithm for the Optimal Design of Integrated Sites Under Uncertainty	2
<i>Sebastian Terrazas-Moreno, Ignacio E. Grossmann, John Wassick, Scott J. Bury</i>	
An Overview of CAST Division Activities	4
<i>Scott E. Keeler</i>	
On-Line Methods to Improve Safety and Performance of Polymerization Reactors	5
<i>Klaus-Dieter Hungenberg II</i>	
Novel, Hybrid, Blood Flow Simulations within Large Arterial Vessels	6
<i>Antony N. Beris, David A Johnson, Ulhas P. Naik</i>	
Numerical and Analytical Coarse-Graining Strategies Based On Relative Entropy Minimization	7
<i>M. Scott Shell, Todd Smith</i>	
A Systematic Coarse-Graining Method to Predict the Structure and Properties of Polymer-Nanoparticle Mixtures	8
<i>Youthachack Landry Khounlavong, Venkat Ganesan, Victor Pryamitsyn</i>	
Systematic Multiscale Modeling of Polymer/Fullerene Bulk Heterojunctions for Photovoltaic Applications	9
<i>David M. Huang, Adam J. Moulé, Roland Faller</i>	
A Coarse-Grained Model for Explicit Solvation of DNA by Water and Ions	10
<i>Robert C. Demille, Thomas E. Cheatham III, Valeria Molinero</i>	
Twist Propagation in Two-Nucleosome Arrays: Monte Carlo Simulations and Theory	11
<i>Martin Kenward, Irina V. Dobrovolskaia, Gaurav Arya</i>	
Raft Registration Across Bilayers by Coarse-Grained Molecular Dynamics	12
<i>Diego A. Pantano, Michael L. Klein, Preston B. Moore, Dennis E. Discher</i>	
Multiscale Molecular Modeling to Investigate the Aggregation of Polyamidoamine Dendrimers in Solution	13
<i>Seung Ha Kim, Monica H. Lamm</i>	
Model and Computational Reduction for Molecular Dynamics of Polymer Systems	14
<i>Yuzhen Xue, Peter Ludovice, Martha Grover</i>	
Estimation Methods for Battery State of Charge Determination	16
<i>Edward P. Gatzke</i>	
Globally Optimal Nesting of Irregular Shapes Into a Limited Resource	17
<i>Ruth Misener, Christodoulos A. Floudas</i>	
Development of a New Homotopy Method for Finding All Real Roots of Systems of Unconstrained Nonlinear Algebraic Equations	19
<i>Saeed Khaleghi Rahimian, Farhang Jalali, J. D. Seader, Ralph E. White</i>	
Programming Paradigms for Multiphysics Simulation at Petascale and Exascale	27
<i>James C. Sutherland</i>	
Progress On a Fully-Implicit Stabilized Finite Element Formulation for Resistive Magnetohydrodynamic Systems	28
<i>Roger P. Pawlowski, John N. Shadid, Eric C. Cyr, Luis Chacon</i>	
Predicting Thermodynamic Equilibrium Composition in Steam Methane Reforming Reaction by Iteration	29
<i>Yuguo Wang, Cemal Ercan</i>	
Global Optimization of a Special Class of Nonlinear Problems	34
<i>João Teles, Pedro Castro, Henrique A. S. Matos</i>	
Exploiting Vector Space Properties to Strengthen the Relaxation of Bilinear Programs Arising in the Global Optimization of Process Networks	36
<i>Juan P. Ruiz, Ignacio E. Grossmann</i>	
Efficient Parallel Optimization On Emerging Computational Architectures	39
<i>Sean Legg, Yu Zhu, Carl D. Laird</i>	
Globally Optimal TAC for Compressors and Coolers in Series	40
<i>Jeremy A. Conner, Vasilios I. Manousiouthakis</i>	
Global Optimization of a Class of Large Scale Process Operations Problem through Dual Decomposition	41
<i>Zukui Li, Marianthi Ierapetritou</i>	

Large-Scale Global Optimization of Generalized and Extended Pooling Problems: Methods and Computational Tools	43
<i>Ruth Misener, Jeffrey P. Thompson, Christodoulos A. Floudas</i>	
Novel Relaxations for Global Optimization	46
<i>Nick Sahinidis, Aida Khajavirad</i>	
A Discretization Approach for the Optimal Design of Mass Integration Networks of Eco-Industrial Parks	47
<i>Eusiel Rubio-Castro, José María Ponce-Ortega, Mahmoud M. El-Halwagi, Medardo Serna-González, Arturo Jiménez-Gutiérrez</i>	
A Superstructure-Based Process Synthesis Framework.....	56
<i>Carlos A. Henao, Christos T. Maravelias</i>	
An Iteratively Refined Distillation Design Method	58
<i>Angelo Lucia, Chris Hassan</i>	
Towards the Integrated Design of Processes and Solvent Blends for CO₂ Capture	59
<i>Niall Mac Dowell, Amparo Galindo, George Jackson, Claire Adjiman</i>	
Integrated Design and Control of Heat Exchanger Networks (HENs) for Multiperiod Operation	61
<i>K. J. Venkatesh, Sridharakumar Narasimhan, Shankar Narasimhan</i>	
A Systematic State Space Superstructure Based Algorithm for the Optimal Design of Azeotropic Distillation Processes	63
<i>Xiao Yang, Hong-Guang Dong</i>	
An Overview of Tom Edgar's Contributions to Chemical Process Systems Engineering	71
<i>B. Wayne Bequette, Dale E. Seborg</i>	
Modeling and Control of a Radiation Therapy Couch	72
<i>Thomas J. McAvoy, Kate Malinowski, M. Ali Yousuf, Warren D. D'Souza</i>	
Controlling Large-Scale Systems with Distributed Model Predictive Control	75
<i>James B. Rawlings</i>	
Quality-Relevant Process Monitoring	76
<i>S. Joe Qin</i>	
Process Systems Engineering in Pharma Product Development (to be revised)	77
<i>Gintaras V. Reklaitis</i>	
Critical Review of 30 Years of Adaptive Control.....	78
<i>B. Erik Ydstie</i>	
Implementation of Novel Integrated Pharmaceutical Processes: A Model-Based Approach.....	79
<i>Alicia Román Martínez, Rafiqul Gani, John M. Woodley</i>	
Design Space of Pharmaceutical Processes Using Data-Driven Based Methods	80
<i>Fani Boukouvava, Fernando J. Muzzio, Marianthi G. Ierapetritou</i>	
Model Based Control of Drug Substance Particle Size to Ensure Drug Product Uniformity	83
<i>Jon Hilden, Mark Schrad, Jessica T. Sloan, Jennifer Kuehne-Willmore, Timothy Kramer</i>	
Modeling the Roll Compaction Process Using Finite Element Analysis	84
<i>Ariel Muliadi, Carl R. Wassgren, James D. Litster</i>	
Application of Model Based Drug Substance Particle Size Control in Drug Product Development	86
<i>Mark Schrad, Jon Hilden, Jessica T. Sloan, Jennifer Kuehne-Willmore</i>	
Investigation of a Tablet Coating Process Using a Multi-Model Simulation Approach	87
<i>Daniele Suzzi, Gregor Toschkoff, Daniel Machold, Johannes Khinast</i>	
Reduction of Stochastic On-Lattice Chemical Kinetics Models to Well-Mixed Descriptions Via Singular Perturbation	88
<i>Michail Stamatakis, Dionisios G. Vlachos</i>	
A Coarse-Grained Approach to Agent-Based Computations: Coarse Bifurcation Analysis, Rare Event Analysis, and a Patch Dynamics Scheme	89
<i>Ping Liu, William Gear, Giovanni Samaey, Ioannis G. Kevrekidis</i>	
A Continuum-Atomistic Hybrid Simulation of Droplet Spreading On a Flat Solid Surface.....	92
<i>Hongfei Wu, Kristen A. Fichthorn, Ali Borhan</i>	
Multiphysics Simulation of Interfacial Phenomena by Fluctuating Hydrodynamics	93
<i>Barry Shang, Jhih-Wei Chu</i>	
Evaluation of Metamodeling Techniques for Discrete-Time Approximations	94
<i>Andres F. Hernandez Moreno, Martha A. Grover</i>	
A Novel Computational Architecture for Construction and Execution of Modular, Multiscale, Multi-Algorithmic Dynamical Models	96
<i>Leonard A. Harris, Justin S. Hogg, Mohammad Fallahi-Sichani, Jennifer J. Linderman, Denise E. Kirschner, James R. Faeder</i>	
Managing Multi-Scale Modeling Issues in Chemical Engineering — A Computer-Aided Framework.....	97
<i>Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani</i>	

Use of the Ornstein-Zernike Percus-Yevick Equation to Extract Interaction Potentials From Pair Correlation Functions	99
<i>Qifei Wang, David Keffer, Donald M. Nicholson, Brock Thomas</i>	
Field Biased Molecular Simulation Technique for Complex Fluids	100
<i>Amir Vahid, Jrichard Elliott</i>	
Spatial Updating Monte Carlo in the Great Grand Canonical Ensemble.....	101
<i>G. Orkoulas</i>	
Systematic Identification of Coarse Variables in Biomolecular Systems through Dimensionality-Reduction Tools: Reconstruction and Navigation of Free-Energy Landscapes	103
<i>Miguel A. Amat, Lilia V. Bravewolf, Andrew L. Ferguson, Gerhard Hummer, Ioannis G. Kevrekidis</i>	
Dimerization of Protegrin-1 Peptides in Different Environments	105
<i>Victor Vivcharuk, Yiannis N. Kaznessis</i>	
A Multi-Scale Approach to Modeling Aqueous Electrolyte Mixtures at High Pressure.....	106
<i>Angelo Lucia, Brian Bonk, David Freeman, Jae W. Lee, Richard Waterman</i>	
Multi-Scale Modeling of Polymer Electrolyte Membrane Fuel Cells.....	107
<i>Robert L. Smith, Pil Seung Chung, Jan Steckel, Lorenz T. Biegler, Myung S. Jhon</i>	
Global Optimization of Discontinuous Functions	109
<i>Achim Wechsung, Paul I. Barton</i>	
Deterministic Global Optimization of Semi-Infinite Programs	111
<i>Alexander Mitsos</i>	
Real-Time Water Management in Power Plants and Implications in Electricity Markets	113
<i>Juan M. Salazar, Urmila Diwekar, Emil Constantinescu, Victor M. Zavala</i>	
A New MILP Model for the 2-D Strip Packing Problem.....	114
<i>Pedro Castro, José F. Oliveira</i>	
Robust Dual Global Optimization Algorithms for the Determination of Fluid Phase Equilibria with the SAFT Equation of State	116
<i>Frances Pereira, Amparo Galindo, George Jackson, Claire Adjiman</i>	
Global Optimization of Sizing Problem in Pipe Networks	118
<i>Arvind Raghunathan</i>	
Pyomo: Python Optimization Modeling Objects.....	119
<i>William Hart, Carl D. Laird, John D. Siirola</i>	
Hartree Fock Self-Consistent Calculations: Global Optimization of Electronic Structure.....	120
<i>Keith Zorn Jr., Nick Sahinidis</i>	
Optimal Design of Extractive Distillation Systems Using a Two-Level Approach	122
<i>Pablo Garcia-Herreros, Ivan D. Gil, Gerardo Rodriguez, Jorge M. Gomez</i>	
Coupling Water-Reuse Network Designs for Agile Manufacturing	125
<i>Jie Fu, Chuanyu Zhao, Qiang Xu</i>	
Whole-Plant Design Optimization	126
<i>Alejandro Cano, Hilario Martin Rodriguez</i>	
Optimization-Based Synthesis, Design and Evaluation of Process Concepts for Production of Pure Enantiomers	127
<i>Malte Kaspererit, Javier Garcia Palacios, Subramanian Swernath, Andreas Seidel-Morgenstern, Achim Kienle</i>	
A Systematic Framework for Simultaneous Product and Flowsheet Design	128
<i>Susilpa Bommareddy, Nishanth Chemmangattuvalappil, Mario Richard Eden</i>	
Least-Squares Finite Element Methods for Large Scale Incompressible Flows	129
<i>Tate Tsang, X. Ding, Q. Y. Jiang</i>	
Tom Edgar's Contributions to the Semiconductor Industry: From Controlling Processes to Technology Development	130
<i>Stephanie Watts Butler</i>	
Estimation of the State of Model Predictive Control	131
<i>Thomas A. Badgwell</i>	
Tom Edgar's Contributions to Modeling and Control In Refining (to be revised)	132
<i>Tyler A. Soderstrom</i>	
Global Sensitivity Analysis Procedure Accounting for Effect of Available Experimental Data	133
<i>Yunfei Chu, Zuyi (Jacky) Huang, Mitchell Serpas, Juergen Hahn</i>	
Rebuttal	134
<i>Thomas F. Edgar</i>	
An Infinite Horizon Formulation of NMPC with Economic Objectives	135
<i>Rui Huang, Lorenz T. Biegler</i>	
Simultaneous Constrained Moving Horizon State Estimation and Model Predictive Control by Multi-Parametric Programming	136
<i>Anna Voelker, Konstantinos Kouramas, Efstratios N. Pistikopoulos</i>	

Control Structure Adaptation for Linear Constrained Systems	138
<i>Sridharakumar Narasimhan, Sigurd Skogestad</i>	
Reduced Linear Model Predictive Control for Non-Linear Distributed Parameter Systems	140
<i>Ioannis Bonis, Constantinos Theodoropoulos</i>	
Market Responsive Control: A Second Order Approach to Economic Based Controller Design	142
<i>Donald J. Chmielewski, Ming-Wei Yang, David Mendoza-Serrano</i>	
An Adaptive Predictor Corrector Strategy for Control of Nonlinear Hybrid Process Systems	143
<i>Ye Hu, Nael H. El-Farra</i>	
Extended SBX-RCGA Neural Network-Based Multi-Model Predictive Control for Wastewater Neutralization Process	145
<i>Weiting Tang, M. Nazmul Karim</i>	
Rapid Prototyping of Reverse Osmosis Processes Using Data-Driven Models	146
<i>Xavier Pascual, Han Gu, Alex Bartman, Aihua (Richard) Zhu, Anditya Rahardianto, Jaume Giralt, Robert Rallo, Francesc Giralt, Yoram Cohen</i>	
Detailed 3-D Dynamic Analysis of Depressurizing Vessels	147
<i>Zbigniew Urban</i>	
A Dynamic Optimization Approach to the Design of Air Separation Plants	148
<i>Yanan Cao, Christopher L. E. Swartz, Stephane Blouin, Michael Baldea</i>	
Efficient Start-up and Shut-Down Strategies for Simulated Moving Beds by Dynamic Optimization	150
<i>Suzhou Li, Yoshiaki Kawajiri, Joerg Raisch, Andreas Seidel-Morgenstern</i>	
Deterministic Global Optimization of Processes Described by Nonlinear Differential-Algebraic Equations	152
<i>Joseph K. Scott, Paul I. Barton</i>	
Rigorous Global Optimization for Dynamic Systems Subject to Path Constraints	154
<i>Yao Zhao, Mark A. Stadtherr</i>	
Generalization of a Tailored Approach for Dynamic Simulation and Optimization	156
<i>Tilman Barz, Duc Hoang Minh, Harvey Arellano-Garcia</i>	
Robust Nonlinear Model Predictive Control for a Reactor with Runaway Conditions	158
<i>Udo Schubert, Harvey Arellano-Garcia, Andreas Lange, Günter Wozny</i>	
Introduction and Session Objectives	161
<i>Phillip Westmoreland, Peter T. Cummings, Sharon C. Glotzer</i>	
Inventing a New America through Discovery and Innovation in Science, Engineering and Medicine	162
<i>Peter T. Cummings, Sharon C. Glotzer</i>	
Integrated, High Fidelity, Multiscale Process Models for the Process Industries	163
<i>Chau-Chyun Chen</i>	
Petascale High-Fidelity Simulation of Turbulent Reactive Flows: Challenges and Opportunities	164
<i>Jacqueline H. Chen</i>	
Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security	165
<i>John Allison</i>	
Open Discussion On High Performance Computing in Chemical Engineering	166
<i>Sharon C. Glotzer, Peter T. Cummings, Phillip Westmoreland</i>	
Modeling the Effect of Temozolomide On Tumor Progression Using An Agent-Based Lattice-Free Approach	167
<i>Francisco G. Vital-Lopez, Michelle Hutnik, Costas D. Maranas, Antonios Armaou</i>	
A Novel Framework for Beta Sheet Topology Prediction in Purely Beta and Mixed Alpha-Beta Proteins	168
<i>Ashwin Subramani, Yanjie Wei, Christodoulos A. Floudas</i>	
Three-Dimensional Multispecies Nonlinear Tumor Growth	170
<i>Fang Jin, Herman Frieboes, Yaoli Chuang, Steven Wise, John Lowengrub, Vittorio Cristini</i>	
Protein Structure Alignment by Derivative-Free Optimization	171
<i>Shweta B. Shah, Nick Sahinidis</i>	
Bacterial Aerosol Neutralization by Aerodynamic Shocks Using An Impactor System: An Integrated Computational and Experimental Study On B.~Atropheus Spores	172
<i>Patrick R. Sislian, Jesse Rau, Xinyu Zhang, David Pham, Mingheng Li, Lutz Madler, Panagiotis Christofides</i>	
Stochastic Modeling of Biological and Gates	173
<i>Bennett J. Swiniarski, Yiannis Kaznessis</i>	
Dynamics of Erythrocytes in Vascular Vessels Via a Non-Stiff Cytoskeleton-Based Continuum Computational Algorithm	174
<i>Panagiotis Dimitrakopoulos, Walter Dodson</i>	
Integrated Product Design and Control in Manufacturing Processes	175
<i>Qian Gou, Mark D. Wetzel, Babatunde A. Ogunmaike</i>	

Unconstrained Nonlinear State Estimation Applied to PMMA and LLDPE Polymerization Processes	177
<i>Arjun V. Shenoy, Vinay Prasad, Sirish L. Shah</i>	
Landfill Modeling Using Ensemble Kalman Filter	179
<i>Hu Li, S. Joe Qin, Muhammad Sahimi, Theodore Tsotsis</i>	
Output Feedback Mixed H_2/H_∞ Model Predictive Control: Observer Based Approach	181
<i>Aadaleesan Pakkirisamy, Prabirkumar Saha</i>	
Outlier Detection for a Recursive Soft Sensor and Its Application to Digester Control	183
<i>Hector Galicia, Qinghua He, Jin Wang, Russel E. Hodges, Gopal Krishnagopalan, Harry T. Cullinan</i>	
Simulation Studies of Active Control Strategy for Sort-Synchronization of Droplets in a Microfluidic Loop Device Using Model Predictive Control	185
<i>Jeevan Maddala, Babji Srinivasan, Swastika S. Bithi, Siva A. Vanapalli, Raghunathan Rengaswamy</i>	
MPC Performance and Monitoring for a Demethanizer Column in a Natural Gas Processing Unit	186
<i>Alexandre De França Cordeiro, Mauricio Bezerra De Souza Jr.</i>	
Quantitative Structure-Property Relationship Models — A Comparison of Different Methodologies	187
<i>K. M. Yerramsetty, B. J. Neely, K. A. M. Gasem</i>	
Characterization Based Chemical Product Design for the Nanoscale	188
<i>Charles C. Solvason, Nishanth Chemmangattuvalappil, Mario Richard Eden</i>	
Managing the Complexity in Liquid Formulation Design	191
<i>Elisa Conte, Rafiqul Gani</i>	
Use of Aggregation Predictions in the Design of Protein Formulations	193
<i>Brock C. Roughton, Anthony I. Pokphanh, T. Steele Reynolds, J. Laurence, E. M. Topp, K. V. Camarda</i>	
Design of Base Fluids for High Pressure/High Temperature Drilling	194
<i>Apurva Samudra, Nick Sahinidis</i>	
Structure-Property Relations for the Design of Organic Glasses for Organic Electronics and Nanolithography	196
<i>Richard A. Lawson, Clifford L. Henderson</i>	
Biorefinery Network Design Under Uncertainty	197
<i>Korin Reid, Matthew Realf</i>	
Robust Design of Subsea Production Facilities	198
<i>Matthew D. Stuber, Paul I. Barton</i>	
Solution Strategies for Multistage Stochastic Programming in the Planning of Process Networks Under Endogenous Uncertainties	200
<i>Vijay Gupta, Ignacio E. Grossmann</i>	
Bayesian Experimental Designs: A Decision Theoretic Framework Applied to Industrial Case Studies	203
<i>Kenneth T. Hu, Gregory J. McRae</i>	
A Robust Method for Process Design Under Uncertainty	204
<i>Adekunle M. Adeyemo, Gregory J. McRae</i>	
Optimal Experimental Design Under Uncertainty	206
<i>Tilman Barz, Harvey Arellano-Garcia, Günter Wozny</i>	
Optimization of Seawater Cooling in Power Plants	218
<i>Abdullah S. Bin Mahfouz, Selma Atilhan, Patrick Linke, Ahmed Abdel-Wahab, Bill Batchelor, Mahmoud El-Halwagi</i>	
A Systematic Methodology for Sustainability Assessment in the Design of Chemical/Energy Production Systems	219
<i>Xiang Li, Helen Lou, Anand Zanwar, Abhishek Jayswal</i>	
Process Design for Hybrid Process Combining Steam Reforming with Dry Methane Reforming to Reuse Carbon Dioxide as a Raw Material	220
<i>Youngsub Lim, Chul-Jin Lee, In-Hyoun Song, Chonghun Han</i>	
Including Ecosystem Goods and Services in Engineering Process Design	221
<i>Geoffrey F. Grubb, Bhavik R. Bakshi</i>	
Optimal Integration of Industrial Scale Biomass Feedstock Based Chemical Processes in the Petrochemical Complex of the Lower Mississippi River Corridor	222
<i>Debalina Sengupta, Ralph W. Pike, Thomas A. Hertwig, Helen H. Lou</i>	
A Multiscale and Multiobjective Optimization Based Approach for Environmentally Conscious Process Design	228
<i>Vikas Khanna, Bhavik R. Bakshi</i>	
Utilization of Municipal Wastewater In Thermoelectric Power Production for Freshwater Minimization	230
<i>Michael E. Walker, Iman Safari, Ming-Kai Hsieh, David C. Miller, David A. Dzombak, Hamid Arastoopour, Javad Abbasian</i>	
Agent-Based Modeling of Angiogenesis and Effects of Synthetic Biogel Scaffold Properties	253
<i>Arsun Artel, Hamidreza Mehdizadeh, Eric M. Brey, Ali Cinar</i>	

Design and Control of a Closed-Loop Neural Prosthesis	255
<i>Gautam Kumar, Vikram Aggarwal, Nitish V. Thakor, Marc H. Schieber, Mayuresh V. Kothare</i>	
Data-Centric Modeling and Predictive Control for Nonlinear Hybrid Systems, with Application to Adaptive Behavioral Interventions	257
<i>Naresh N. Nandola, Daniel E. Rivera</i>	
Computational Modeling of Ozone Dose Distribution in the Respiratory Tract	260
<i>Banafsheh Keshavarzi, James Ultman, Ali Borhan</i>	
Sensitivity Analysis for Limit-Cycle Oscillating Hybrid Systems	261
<i>Kamil A. Khan, Vibhu P. Saxena, Paul I. Barton</i>	
Design of PLGA Microparticle Drug Delivery Systems Using a Reaction-Diffusion Model	263
<i>Ashlee N. Ford, Daniel W. Pack, Richard D. Braatz</i>	
Optimal Therapy for a Pathogenic Disease: A Stochastic Optimal Control Approach	264
<i>Urmila Divekar, Vicente Rico-Ramirez, Guillermo Gonzalez-Alatorre, Oliva Ramirez-Enriquez</i>	
Nonlinear Model-Predictive Control of An Industrial Polymerization Reactor In the Laboratory	265
<i>Arndt Hartwich, Lynn Würth, Jens Bausa, Nina Paula Salau, Fady Assassa, Wolfgang Marquardt</i>	
Modeling and Control of Interpenetrating Polymer Network Process	266
<i>Weijie Lin, Lorenz Biegler, Annette Jacobson</i>	
Decentralized Multi-Agent Control of MWD in RAFT Polymerization CSTR Networks	267
<i>M. Derya Tetiker, Derya Demirel, F. Teymour, A. Cinar</i>	
Non-Isothermal Blown Film Extrusion Including Crystallization: Instabilities, Multiplicities, and Mapping of Stable Operating Regions	270
<i>J. Carl Pirkle Jr., Richard D. Braatz</i>	
Modeling and Control of End-User Polymer Properties in Gas-Phase Polymerization Reactors	273
<i>Min Zhang, John R. Parrish, Ping Cai</i>	
Macroscopic Mechanistic Modeling Studies of Self-Initiated High-Temperature Polymerization of Alkyl Acrylates	290
<i>Sriraj Srinivasan, Thomas Rier, George A. Kalfas, Christopher Bruni, Michael C. Grady, Masoud Soroush</i>	
Gel Time Prediction in Multifunctional Acrylates	291
<i>Aparna Boddapati, Martha Grover, Clifford Henderson</i>	
Efficient Strategies for Coupling Multi-Scale Models for Bulk Crystal Growth	293
<i>Andrew Yeckel, Jeffrey J. Derby</i>	
Accelerated Simulation of Surface Pattern-Forming Systems Via Hierarchical Multi-Scale and Mesoscopic Modeling	295
<i>Nasser Mohieddin Abukhdeir, Dion G. Vlachos</i>	
Multiscale Simulation of Nanofeature Evolution in Atomic Layer Deposition Processes	296
<i>Raymond A. Adomaitis</i>	
Analysis of the Fluid Flow of Czochralski Crystal Growth Process Using Lagrangian Coherent Structures	297
<i>Stevan Dubljevic, Mojtaba Izadi</i>	
Multi-Scale Modelling and Simulation of Catalytic Microreactors	299
<i>Bostjan Hari, Constantinos Theodoropoulos</i>	
Modeling and Control of Aggregate Surface Roughness and Slope in Thin Film Growth for Light Trapping Optimization	301
<i>Gangshi Hu, Jianqiao Huang, Gerassimos Orkoulas, Panagiotis D. Christofides</i>	
Multiscale Hierarchical Design of Polymer Nanocomposite Coatings	303
<i>Jie Xiao, Yinlun Huang</i>	
Extensions to the Resource-Task Network	304
<i>Jeff Ferrio, John Wassick</i>	
A General Framework for Chemical Process Scheduling	313
<i>Arul Sundaramoorthy, Christos T. Maravelias</i>	
A Novel Technique for Prediction of Time Points in Scheduling of Multipurpose Batch Plants	316
<i>Esmael Reshid Seid, Thokozani Majazi</i>	
Optimizing Production Planning Using High Performance Computing	318
<i>Dimitrios Varvarezos</i>	
On the Solution of Batch Process Scheduling MIP Models	319
<i>Arul Sundaramoorthy, Christos T. Maravelias</i>	
Rolling Horizon Based Planning and Scheduling Integration with Production Capacity Consideration	322
<i>Zukui Li, Marianthi Ierapetritou</i>	
Introduction and Objectives of the Session	324
<i>Jim Davis, Thomas F. Edgar</i>	
Smart Process Manufacturing - Capital Programs and Industry Operations	325
<i>James B. Porter Jr.</i>	

Unit Operations for Smart Nanomanufacturing	326
<i>Roger T. Bonnecaze</i>	
Sustainability and Systems Engineering: Reducing the Carbon Footprint of Chemical Plants	327
<i>Jeffrey J. Siirola</i>	
Automation for Smart Manufacturing--Trends and Technologies	328
<i>Tariq Samad</i>	
Open Discussion On Smart Manufacturing	329
<i>Thomas F. Edgar, Jim Davis</i>	
Mechanisms of Self Diffusion at Cu-Nb Semicoherent Interfaces	330
<i>Kedarnath Kolluri, Michael J. Demkowicz</i>	
Preliminary Efforts in the Simulation of Molding of a Polypropylene Melt Reinforced with Long Glass Fibers Using Transient Shear Rheology	331
<i>Kevin C. Orman, Don Baird, Peter Wapperom</i>	
A Hybrid Model for Electrorheological Fluids	332
<i>Sesha Hari Vemuri, Pil Seung Chung, Dehee Kim, Myung S. Jhon</i>	
Multi-Scale Modeling of Ionic Liquid Dispersed Nanoparticles in Epoxy Resin	334
<i>James A. Throckmorton, Giuseppe R. Palmese</i>	
Heat Transfer in Nanocomposites at High Volume Fraction	335
<i>Khoa Bui, Brian P. Grady, Hai M. Duong, Dimitrios V. Papavassiliou</i>	
Optimization of Biodiesel Production Under Uncertainty	336
<i>Sheraz Abbasi, Urmila D. Diwekar</i>	
New Strategies for Polygeneration: Hybrid Natural Gas Reforming and Coal Gasification Techniques for Production of Methanol, Electricity, and Fischer-Tropsch Fuels	339
<i>Thomas A. Adams II, Paul I. Barton</i>	
An Integrated Multi-Scale Spatiotemporal Modelling Framework for Optimal Design of CO₂ Capture, Transport and Storage Networks	341
<i>Ahmed Alhajaj, Niall Mac Dowell, Murthy Konda, Nilay Shah</i>	
Optimization Studies of An Integrated Gasification Combined Cycle (IGCC) Plant with CO₂ Capture	343
<i>Debangsu Bhattacharyya, Richard Turton, Stephen E. Zitney</i>	
Computer-Aided Selection and Design of Working Fluids for Organic Rankine Cycles	344
<i>Patrick Linke, Mirko Z. Stijepovic, Athanasios I. Papadopoulos</i>	
Estimation of State of Charge of a Lithium-Ion Battery Pack	345
<i>Venkatasailanathan Ramadesigan, Ravi N. Methekar, Sumitava De, Richard D. Braatz, Venkat Subramanian</i>	
Process Development and Techno-Economic Analysis of a Novel Process for MeOH Production From CO₂ Using Solar-Thermal Energy	348
<i>Jiyong Kim, Carlos Henao, Christos Maravelias, James E. Miller, Daniel E. Dedrick, Terry A. Johnson</i>	
Mitigation of Fouling in a Super-Decanter Centrifuge	351
<i>Akiya Kuboyama, Hirofumi Inokuchi, Christiano Wibowo</i>	
Challenges in Low Temperature Process Design	352
<i>Danahe Marmolejo-Correa, Truls Gundersen</i>	
Exergy-Analysis Based Refrigeration System Synthesis at Ethylene Plants	354
<i>Jian Zhang, Yanqin Wen, Qiang Xu</i>	
Fully Automatic Computer-Aided Design and Synthesis of Complex Separation Networks	355
<i>Seon B. Kim, Andreas A. Linninger</i>	
Comparison of Mixing in Rocking Reactors and a Laboratory Dyeing Reactors	356
<i>Srinivas Hanumansetty, Edgar O Rear</i>	
Optimal Synthesis and Design of Three-Phase Separator for Upstream Oil and Gas Processes	357
<i>Rajab Khalilpour, Ali Abbas</i>	
Verified Probability Bounds Analysis around Bifurcations in An Ecosystem Model	358
<i>Joshua A. Enszer, Kate A. Smith, Mark A. Stadtherr</i>	
A Model Reduction Approach to Activated Sludge Systems	360
<i>Mariano Nicolas Cruz Bournazou, Harvey Arellano-Garcia, Günter Wozny, Gerasimos Lyberatos, Costas Kravaris</i>	
Coupling Electroplating Process Design and Operation for Simultaneous Productivity Maximization, Energy Saving, and Wastewater Minimization	362
<i>Chaowei Liu, Qiang Xu</i>	
Heat Integration of the Water-Gas Shift Reaction System for Carbon Sequestration Ready IGCC Process with Chemical Looping	364
<i>Juan M. Salazar, Stephen Zitney, Urmila Diwekar</i>	
Optimization of Power Plant Simulations with Integrated Carbon Capture Systems Using Black-Box Algorithms	365
<i>Alison Cozad, Nick Sahinidis, David C. Miller</i>	

Evaluation of CO₂ Adsorbents for Sorption-Enhanced Water Gas Shift Reaction (SEWGS) Process in Coal Gasification Systems	367
<i>Hong Lu, Yongqi Lu, Massoud Rostam-Abadi</i>	
Transient Studies of An Integrated Gasification Combined Cycle (IGCC) Plant with CO₂ Capture	368
<i>Debangsu Bhattacharyya, Richard Turton, Stephen E. Zitney</i>	
Medically Inspired Benchmarks for Hypoglycemic Event Prediction and Alarming	369
<i>Rebecca A. Harvey, Eyal Dassau, Howard Zisser, Dale E. Seborg, Lois Jovanovic, Francis J. Doyle III</i>	
Understanding Dysregulated Neutrophil Trafficking in Severe Sepsis	375
<i>Sang Ok Song, Justin S. Hogg, Gilles Clermont, Robert S. Parker</i>	
Model-Based Control of Blood Glucose in Intensive Care Unit (ICU) Patients	377
<i>Jing Sun, B. Wayne Bequette, Hyunjin Lee</i>	
Multivariate and Subject-Specific Model for Estimating Future Glucose Concentrations	379
<i>Meriyan Eren-Oruklu, Ali Cinar, Derrick Rollins, Lauretta Quinn</i>	
Annihilation of Cardiac Alternans by Mechanical Perturbation	381
<i>Dipen Deshpande, Stevan Dujic</i>	
A New Mathematical Modeling Approach to Inferring the Distribution of Microbial Resistance From Time-Kill Experiments	383
<i>Pratik Bhagunde, Vincent H. Tam, Michael Nikolaou</i>	
Mathematical Model for Microencapsulation of Cells within Biofunctional PEG Hydrogel	384
<i>Seda Kizilel</i>	
Prediction of Dynamic Particle Size Distribution in Industrial Slurry-Phase Olefin Catalytic Polymerization Loop Reactors	385
<i>Vassilis Touloupides, Vassilis Kanellopoulos, Costas Kiparissides</i>	
Modeling of Precipitation and Dispersion Copolymerization of Fluorinated Monomers in Supercritical Carbon Dioxide	386
<i>Liborio Ivano Costa, Giuseppe Storti, Massimo Morbidelli, Loredana Ferro, Alessandro Galia, Giuseppe Filardo</i>	
Experimental and Modeling Analysis of Lactic Acid Polycondensation	388
<i>Fabio Codari, Giuseppe Storti, Massimo Morbidelli</i>	
A Full Kinetic Analysis of Ring-Opening Polymerization of L,L-Lactide	390
<i>Yingchuan Yu, Giuseppe Storti, Massimo Morbidelli</i>	
On the Prediction of the Viscoelastic Behavior of Highly-Branched Polymer Chains: A Novel Topological - Rheological Approach	392
<i>Prokopis Pladis, Dimitris Meimaroglou, Apostolos Baltas, Costas Kiparissides</i>	
Simulation of Chain-Length Differentiated Properties in High-Pressure High-Temperature Ter-Polymerization	394
<i>Markus Busch, Katrin Becker</i>	
Progress in the Solution of the Equations for the Full Molecular Weight Distribution in Addition Polymerization by Direct Techniques	396
<i>Ivan Zapata Sr., Antonio Flores-Tlacuahuac, Ramiro Infante-Martinez, Enrique Saldivar-Guerra</i>	
On the Combinatorial Properties of Discrete-Time Production Planning and Scheduling MIP Models for Continuous Processes	397
<i>Konstantinos Papalamprou, Christos T. Maravelias</i>	
Time Representations and Mathematical Models for Process Scheduling Problems	399
<i>Sylvain Mouret, Ignacio E. Grossmann, Pierre Pestyiaux</i>	
A New Modeling and Global Optimization Approach for Scheduling of Crude Oil Operations	402
<i>Jie Li, Ruth Misener, Christodoulos A. Floudas</i>	
A Solution Strategy for Large-Scale Nonlinear Petroleum Refinery Planning Models	406
<i>Omar J. Guerra, Ariel Uribe Rodriguez, Sandra Milena Montagut, Laura Andrea Duarte, Javier David Angarita</i>	
Optimal Scheduling of An Industrial Food Manufacturing Facility	407
<i>Matthew Hazaras, Christopher L. E. Swartz, Thomas E Marlin</i>	
On Computational Performance of Big-M Formulations in Scheduling of Multipurpose Batch Plants	409
<i>Thokozani Majozi, Esmael R. Reshid</i>	
Framing Workshop Objectives for Determining AIChE Institute Roles In Simulation Based Engineering and Science	411
<i>Bond Calloway</i>	
The Council on Competitiveness Initiative on US Manufacturing	412
<i>Cynthia McIntyre</i>	
Federal Agency View of Simulation Based Engineering and Science	413
<i>Clark Cooper, Phillip Westmoreland</i>	
Key Information and Data to Inform Discussions about AIChE Institute Roles	414
<i>Jim Davis</i>	

Facilitated Discussion On AIChE Institute Roles In Simulation Based Engineering and Science	415
<i>Bond Calloway, Jim Davis, Phillip Westmoreland</i>	
Robust Fault-Tolerant Control of Distributed Energy Systems	416
<i>Yulei Sun, Nael H. El-Farra</i>	
Simultaneous State Reconstruction and Parameter Identification Using Wavelets	418
<i>Heinz A. Preisig</i>	
Modeling of Tubular High-Pressure Polyethylene Reactors	419
<i>Thomas Herrmann, Markus Busch, Barbara Gall, Dieter Lilge, Gerd Mannebach, Iakovos Vittorias</i>	
Kinetic Modeling and Optimal Control of the Polymerase Chain Reaction	421
<i>Karthikeyan Marimuthu, Raj Chakrabarti</i>	
A Stochastic Approach to Catalyst Optimization: Robust Design of Experiments and Catalysts	422
<i>Chang Jun Lee, Siddhartha Kumar, Vinay Prasad, Jong Min Lee</i>	
Emulsion Copolymerization Process: Mathematical Modeling and Experimental Validation	424
<i>Giovane Marinangelo, Wilson H. Hirota, Reinaldo Giudici</i>	
Negative Selection Algorithm: An Artificial Immune System for Fault Diagnosis In Continuous and Batch Processes	433
<i>Kaushik Ghosh, Rajagopalan Srinivasan</i>	
Monitoring and Diagnosis of An Experimental System	435
<i>Edward P. Gatzke</i>	
Arx-Based Model Predictive Control of Systems with Time Delays	436
<i>Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten B. Jørgensen, John Bagterp Jørgensen</i>	
Efficient Reformulation of Moving Horizon Approach for Nonlinear Constrained State Estimation	437
<i>Vidyashankar Kuppuraj, Raghunathan Rengaswamy, Shankar Narasimhan</i>	
Predicting Efficiency in a Dialyzer: The Use of An Asymptotic Solution and Its Validation	438
<i>Katie Frederick, Jennifer Pascal, Pedro Arce</i>	
Extended SBX-RCGA Neural Network-Based Multi-Model Predictive Control for pH Neutralization Process	439
<i>Weiting Tang, M. Nazmul Karim</i>	
An Efficient Stochastic Programming Framework for Studying the Impact of Seasonal Variation On the Water Consumption of Pulverized Coal (PC) Power Plants	440
<i>Juan M. Salazar, Urmila Diwekar</i>	
Optimal Control of Hydrogen Fill-up	441
<i>Fernando Olmos, Vasilios I. Manousiouthakis</i>	
Wiener Dynamic Modeling Under Inputs with Continuous-Time Stochastic Process Noise	442
<i>Derrick K. Rollins Sr., Dongmei Zhai, Nidhi Bhandari, Rubal Dua, Huaqing Wu</i>	
Plant Friendly Input Design for System Identification	443
<i>Sridharakumar Narasimhan, Raghunathan Rengasamy</i>	
Multivariable Control of Thermal Budget for Rapid Thermal Processing Systems	445
<i>Jyh-Cheng Jeng</i>	
Integrating Economic Targets for Simultaneous Structural and Operational Decision-Making in the Design of the Control Recipe	447
<i>Marta Moreno-Benito, Antonio Espuña, Luis Puigjaner</i>	
Modeling of a Solar Thermal Reactor for Control Purposes	459
<i>Elizabeth Saade, David E. Clough, Alan Weimer</i>	
Relay Feedback Identification for Processes Under Drift and Noisy Environments	460
<i>Jietae Lee, Su Whan Sung, Thomas F. Edgar</i>	
Using the Penalty Immersed Boundary Method to Model the Interaction of Filiform Hairs On Crickets	461
<i>Eric D. Gordon, Jeffrey J. Heys</i>	
A Stochastic Ensemble Model of Human Endotoxemia	469
<i>Jeremy D. Scheff, Steven E. Calvano, Stephen F. Lowry, Ioannis P. Androulakis</i>	
A Generalized Stochastic Model for Bacterial Disinfection: Non-Linear Approach	473
<i>Andres Argoti, L. T. Fan, S. T. Chou</i>	
Parameter Estimation In Global Pharmacokinetic Models for Drug Delivery	474
<i>Andrej Mošat, Eric Lueshen, Cierra Hall, Andreas A. Linninger</i>	
Modeling and Optimization of Biosensors Exploiting Restriction Fragment Length Polymorphism	476
<i>Zhichao (Evan) Zhou, Jeffrey Kantor</i>	
Electromigration-Driven Surface Morphological Stabilization of a Coherently Strained Heteroepitaxial Thin Film	477
<i>Georgios I. Sfyris, Rauf M. Gungor, Dimitrios Maroudas</i>	

A New Discretization Approach for Solving the Pooling Problem	478
<i>Fabrizio Nápoles-Rivera, Viet Pham, José María Ponce-Ortega, Arturo Jiménez-Gutiérrez, Mahmoud M. El-Halwagi</i>	
Ontology Controlled Optimization in Process Synthesis Applications	486
<i>Du Du, Franjo Cecelja, Antonis Kokossis</i>	
Implementation of Distributed Optimisation Algorithm On Computer Grid	488
<i>Du Du, Franjo Cecelja, Antonis Kokossis</i>	
An Alternative Superstructure and Solution Strategies for Global Optimization of Heat Exchanger Networks	489
<i>Milos Bogataj, Zdravko Kravanja</i>	
Optimization of Reactive Semi-Batch Distillation Under Uncertainty Parameters Using Bayesian Network	498
<i>Ali Vahidi, Farhang Jalali Farahani, Majid Nili Ahmadabadi</i>	
Production Optimization of Sulphur Free Diesel Oil Using Ant Colony Technique	506
<i>Mohamad Reza Esmailynasab, Farhang Jalali Farahani, Navid Mostoufi</i>	
A New Approach to Model Identification In E. Coli Fed-Batch Fermentations	513
<i>Mariano Nicolas Cruz Bournazou, Harvey Arellano-Garcia, Peter Neubauer, Günter Wozny</i>	
Quantifying Polymer Structural Component Evolution Using Scattering Data and Mixed-Integer Network Component Analysis	514
<i>Ian Tolle, Lealon L. Martin</i>	
Flow Rate Data Estimation for LNG Terminal Pipeline	515
<i>Sangho Lee, Youngsub Lim, Chun-Jin Lee, Chansaem Park, Chonghun Han</i>	
Visualizing Industrial Multivariable Control Constraints In Operations	516
<i>M. R. Islam, Peyton C. Richmond</i>	
Stop-of-Supply Characterization as a Metric to Improve Operations in a Chemical Supply Chain	529
<i>Pedro Huíztzil-Meléndez, Angel Soriano</i>	
On the Detection of Valve Non-Linearities in Closed Loop Linear Systems	544
<i>Babji Srinivasan, Ulaganathan Nallasivam, Raghunathan Rengaswamy</i>	
Empirical Model Synthesis From Data through Genetic Programming	545
<i>Ying Zhang, Aydin Sunol</i>	
Re	546
<i>Abraham Lee</i>	
A Continuous and Smooth Function for Similarity Measure in Quantitative Process Trend Classification	547
<i>Mano R. Maurya</i>	
Detailed Dynamic Modeling and Simulation of Flare Networks	548
<i>James Marriott, Rodrigo Blanco-Gutierrez</i>	
A Screening Method to Find An Optimal Draw Solute for Forward Osmosis Desalination	549
<i>Tae-Woo Kim, Young Kim, Choamun Yun, Hong Jang, Doyeon Lee, Sunwon Park</i>	
A MSPC Technique for Identifying Biases in Industrial Processes	550
<i>Marco Cedeño, Rubén Galdeano, Leandro Rodriguez, Juan Elwart, Mabel C. Sanchez</i>	
Production Planning, Scheduling, and Debottlenecking Practices in the Biopharmaceutical Industries	556
<i>Charles Siletti, Demetri Petrides</i>	
A Comprehensive and General Class for Solving Nonlinear Model Predictive Control and Dynamic Optimization	557
<i>Flavio Manenti, Nádson M. N. Lima, Lamia Zuniga Linan, Guido Buzzi-Ferraris</i>	
Coupling Performing Numerical Libraries and Detailed Simulators to Accurately Infer/Reconcile Stack Emissions of Incinerator Systems	567
<i>Andrea Cagnacci, Flavio Manenti, Stefano Signor, Maria Grazia Grottoli, Paolo Fabbri, Lucio Molinari</i>	
Two-Time Scale Unscented Kalman Filters for Nonlinear State Estimation with Time-Delayed Measurements. Application to Polymer Processes	577
<i>Rubén Galdeano, Marco Cedeño, Mariano Asteasuain, Mabel C. Sanchez</i>	
Real-Time Monitoring, Fault Detection and Diagnosis for City Gas Pipe Networks	588
<i>Dongil Peter Shin, Yountae Lee</i>	

Volume 2

Systematic Design of An Acetaldehyde Process	589
<i>Deenesh Babi, Jason Price, Rafiqul Gani</i>	
Molecular Design of Biofuel Additives for Feedstock Flexibility	671
<i>Subin Hada, Charles C. Solvason, Mario Richard Eden</i>	
A Systematic Assessment of Carbon-Free Hydrogen Production through Vanadium-Chlorine Thermochemical Cycles	673
<i>Ryan J. Andress, Lealon L. Martin</i>	
Design of An Expert System for a Crude Oil Distillation Column with Bayesian Belief Network	674
<i>Arash Dolatabadi, Farhang Jalali Farahani, Majid Nili Ahmadabadi, Navid Mostoufi</i>	
A State-Space-Based MINLP Formulation for Integrated Separation Network Design	683
<i>Lijuan Li, Ruijie Zhou, Hong-Guang Dong</i>	
Optimal Energy Polygeneration System Design Under Different Economic Scenarios	692
<i>Yang Chen, Thomas A. Adams II, Paul Barton</i>	
Optimization of a Solar-Thermal Cogeneration Plant	693
<i>Amin Ghobeity, Alexander Mitsos</i>	
Design of High-Efficiency Photocatalytic System for CO₂ Reduction Using Novel Photocatalytic Organic-Inorganic Porous Hybrids	695
<i>Sanjay Adhikari, Oshadha Ranasingha, Hui Zhang, James P. Lewis, Xingbo Liu, Xiaodong Shi</i>	
Multi-Product Reactor to Pyrolysis of Solid Wastes	696
<i>Ana Rosa Costa-Muniz Sr., L. A. R. Muniz, P. Homrich</i>	
Sustainability Assessment of Industrial Systems Under Uncertainty: A Fuzzy-Logic-Based Approach to Short-to-Mid-Term Predictions	697
<i>Cristina Piluso, Zheng Liu, Jennifer Huang, Yinlun Huang</i>	
Integrated Process and Molecular Design for Reactive Systems	698
<i>Nishanth Chemmangattuvalappil, Charles C. Solvason, Susilpa Bommarreddy, Mario Richard Eden</i>	
Feedback Control of Distributed Processes Using Adaptive Proper Orthogonal Decomposition with Partial Information; The Gappy APOD Method	N/A
<i>Sivakumar Pitchaiah, Antonios Armaou</i>	
A Simulation Study On SCR (Steam Carbon Dioxide Reforming) Process Optimization for Fischer-Tropsch Synthesis	701
<i>Yong Heon Kim, Kee Young Koo, Ji Han Bae, Jae Ho Kim</i>	
Multiobjective Synthesis of Heat Exchanger Networks Minimizing the Cost and the Environmental Impact	702
<i>Lizbeth Anabel López-Maldonado, José María Ponce-Ortega, Juan Gabriel Segovia-Hernández</i>	
Optimal Location of Industrial Plants Considering Economic and Environmental Issues Simultaneously	710
<i>Luis Fernando Lira-Barragán, José María Ponce-Ortega, Medardo Serna-González, Mahmoud M. El-Halwagi</i>	
Optimization of CO₂ Capture Process with Aqueous Amine Using Response Surface Methodology	718
<i>Aroonsri Nuchitprasittichai, Selen Cremaschi</i>	
Optimal Design and Planning of Integrated Bioethanol-Sugar Supply Chains with Economic and Environmental Concerns. A Case Study of the Sugar Cane Industry in Argentina	719
<i>Andrei Kostin, Gonzalo Guillén-Gosálbez, Fernando Daniel Mele, Laureano Jiménez</i>	
Identification of Optimal Filtration Networks for Recreational Water Use	721
<i>David M. Follansbee, Lealon L. Martin, John Paccione</i>	
Optimization of Regional Water Desalination and Supply Networks	722
<i>Selma Atilhan, Abdullah Bin Mahfouz, Mahmoud M. El-Halwagi, Patrick Linke, Ahmed Abdel-Wahab</i>	
A Property Based Approach to Molecular Design in Reactive Systems	723
<i>Nishanth Chemmangattuvalappil, Charles C. Solvason, Susilpa Bommarreddy, Mario Richard Eden</i>	
Multiscale Chemical Product Design Using Chemometric Techniques in a Reverse Problem Formulation	724
<i>Charles C. Solvason, Nishanth Chemmangattuvalappil, Mario Richard Eden</i>	
Multi-Scale Modeling of Head Disk Interface	727
<i>Pil Seung Chung, Robert L. Smith, Sessa Hari Vemuri, Myung S. Jhon, Lorenz T. Biegler</i>	
Optimal Planning of Biodiesel Supply Chain in Argentina with Alternative Oil Sources	729
<i>Federico Andersen Sr., Facundo Iturmendi, Susana N. Espinosa, Maria Soledad Diaz</i>	
Process Modeling and Integration of Fischer-Tropsch Fuels Production Strategies	730
<i>Wei Yuan, Mario Richard Eden</i>	
An Integrated Approach to the Design and Operation of Solar-Driven Absorption Refrigeration Systems	731
<i>Eman Tora, Mahmoud M. El-Halwagi</i>	

Property Based Methods for Flowsheet and Molecular Synthesis	732
<i>Susilpa Bommareddy, Nishanth Chemmangattuvalappil, Mario Richard Eden</i>	
Reduced-Order Models for Lithium-Ion Batteries: Comparison of Proper Orthogonal Decomposition Versus Reformulated Models	733
<i>J. Carl Pirkle Jr., Venkatasailanathan Ramadesigan, Ravi N. Methekar, Richard D. Braatz, Venkat Subramanian</i>	
Computing in Chemical Engineering Education: From Mainframes to Main Street	735
<i>Duncan A. Mellichamp</i>	
POLYMATH — The Present, the New DIPPR Database Option and the Future of This Popular CACHE Numerical Problem-Solving Package	743
<i>Michael B. Cutlip, Mordechai Shacham</i>	
A Student Competition to Develop a Chemical Engineering App for the Iphone	744
<i>Peter T. Cummings, Clare McCabe</i>	
Energy Modules for the ChE Curriculum	745
<i>Jason M. Keith, Thomas F. Edgar, Gavin P. Towler, H. Scott Fogler, David T. Allen, Darlene Schuster</i>	
Modules for High School Engineering Courses	746
<i>David T. Allen</i>	
ChemSep, COCO and Formula Based Unit Operation Tools	747
<i>Jasper M. Van Baten, Harry Kooijman, Ross Taylor</i>	
Study of the Impact of Biofuels On the Sustainability An Integrated Ecosystem Model	755
<i>Prakash Kotecha, Urmila Divekar, Heriberto Cabezas</i>	
Complexity Analysis of Gasoline and Corn-Ethanol Life Cycle Networks	756
<i>Shweta Singh, Bhavik R. Bakshi</i>	
Assessment of Urban Agriculture as a Means towards Sustainable Food Systems: An Integrated Modeling Approach Involving Stakeholder Behavior	758
<i>Arunprakash T. Karunanithi, Stephen Fisher</i>	
A Systematic Method for Reducing the Number of Objectives in Multi-Objective Optimization: Application to Environmental Problems	759
<i>Gonzalo Guillén-Gosálbez</i>	
Distributed Model Predictive Control of Two-Time-Scale Nonlinear Systems	761
<i>Xianzhong Chen, Jinfeng Liu, David Muñoz De La Peña, Panagiotis D. Christofides</i>	
Evaluating Triple Bottom Line Sustainability of Global Supply Chains Using Dynamic Simulation	763
<i>Peng Cheng Wang, Iskandar Halim, Arief Adhitya, Rajagopalan Srinivasan</i>	
Optimal Design of Bioprocesses with Economic and Environmental Concerns Via a Combined Simulation-Optimization Approach	765
<i>Robert Brunet, Gonzalo Guillén-Gosálbez, José Antonio Caballero, Laureano Jiménez</i>	
Energy Optimization of Bioethanol Production Via Gasification of Switchgrass	767
<i>Mariano Martin, Ignacio E. Grossmann</i>	
Low Temperature Hydrothermal Crystallization for a New TiO₂ Process	770
<i>Keith W. Hutchenson, David R. Corbin, Eugene M. McCarron, Charles C. Torardi, Sheng Li</i>	
Synthesis of Recycle/Reuse Networks Based On Properties Considering Simultaneously Economic and Environmental Concerns	771
<i>José María Ponce-Ortega, Francisco Waldemar Mosqueda-Jiménez, Meadardo Serna-González, Arturo Jimenez-Gutierrez, Mahmoud M. El-Habwagi</i>	
Preliminary Synthesis of Work Exchange Networks	779
<i>M. S. Razib, M. M. F. Hasan, I. A. Karimi</i>	
Utilizing Fossil Fuels Effectively: Applying the Attainable Chemical Processes (ACP) Approach	781
<i>Bilal Patel, Diane Hildebrandt, David Glasser</i>	
Business Development, IP, and Manufacturing Success: Perspectives From Utah's Manufacturing Extension Partnership	782
<i>David Sorensen</i>	
Role of IP In Successful Startups	783
<i>Michael Alder</i>	
An Introduction to IP Law: The Underpinnings of Intellectual Assets	784
<i>Ken Horton</i>	
Cost-Effective Pursuit of IP in a Down Economy	785
<i>Jonathan Lee</i>	
Parameter Estimation for Flexible Fuel Energy Conversion Networks	786
<i>Patrick Mousaw, Jeffrey Kantor</i>	
Dynamic Modeling and Control of Heat Recovery Steam Generator and Steam Turbine Units as Part of IGCC Power Plants	788
<i>Priyadarshi Mahapatra, Jing Sun, B. Wayne Bequette</i>	

Minimizing the Utility Cost of An ASU Based On Multi-Scenario NMPC with Economic Objective Function	789
<i>Rui Huang, Lorenz T. Biegler</i>	
Real-Time Model Predictive Control for Energy and Demand Optimization of Multi-Zone Buildings	790
<i>Jingran Ma, S. Joe Qin, Tim Salsbury</i>	
Decentralized Control for Power Systems Subject to Wind Power Variability	792
<i>Juhua Liu, Bruce Krogh, B. Erik Ydstie</i>	
Optimization of Well Placement and Geometry for Tight Natural Gas Production	793
<i>Srimoyee Bhattacharya, Michael Nikolaou</i>	
Stochastic Pooling Problem for Natural Gas Production Network Design and Operation Under Uncertainty	794
<i>Xiang Li, Emre Armagan, Asgeir Tomasgard, Paul I. Barton</i>	
Bayesian Belief Networks (BBNs) for Integration of Parallel Fault Diagnosis Modules Into Supervisory Control Systems	796
<i>Kris Villez, Tim Spinner, Humberto Garcia, Craig Rieger, Raghunathan Rengaswamy, Venkat Venkatasubramanian</i>	
Robust Detection of Mode Transitions in Hybrid Process Systems with Measurement Sampling Constraints	800
<i>Ye Hu, Nael H. El-Farra</i>	
Multi - Agent Based Process Supervisory System for Monitoring Large Scale Chemical Processes	803
<i>Sathish Natarajan, R. Srinivasan</i>	
An Adaptive Framework for Fault Diagnosis with Agent-Based Systems	805
<i>Sinem Perk, Fouad Teymour, Ali Cinar</i>	
Reliability Based Sensor Network Design for Fault Diagnosis	807
<i>Mani Bhushan, Sridharakumar Narasimhan, Raghunathan Rengasamy</i>	
A Recursive Method for Variable Selection Using Principle Component Analysis and Factor Analysis for Identification of System Status in a Commercialized 300kW MCFC Power Plant	809
<i>Hyunseok Chung, Sungwoo Cho, Daeyoun Kim, Hahyung Pyun, Chonghun Han</i>	
Real-Time Monitoring, Fault Detection and Diagnosis for CNG Recharging Stations	810
<i>Yountae Lee, Dongil Peter Shin</i>	
A Decomposition Framework for Scheduling of Refinery Operations Including Logistics	813
<i>Nikisha Shah, M. G. Ierapetritou</i>	
Decision Support for the Routing, Scheduling, & Bunkering of Multi-Parcel Chemical Tankers	816
<i>I. A. Karimi, H. C. Oh, X. Wu</i>	
A Mathematical Programming Framework for Locating Alternative Transportation Fuel Stations On a Large Scale Real-Life Network	818
<i>Aviral Shukla, Joseph F. Pekny, Venkat Venkatasubramanian</i>	
Optimizing the Logistics of Compressed Natural Gas Transportation by Marine Vessels	820
<i>Michael Nikolaou, Michael J. Economides</i>	
A Hybrid Approach for the Exact Solution of the Capacitated Vehicle Routing Problem	822
<i>Chrysanthos E. Gounaris, Panagiotis P. Repoussis, Christos D. Tarantilis, Christodoulos A. Floudas</i>	
Scheduling Multiproduct Pipeline Systems with RTN-Based Formulations	825
<i>Pedro Castro</i>	
A Decision Support Framework for Strategic Decision Assessment of a Sustainable Biorefinery	827
<i>Paritosh K. Sharma, Jose Romagnoli</i>	
Model-Based Optimization of An Algal Bioreactor Coupled to An Anaerobic Digester	829
<i>Elliot T. Cameron, Francis Mairet, Olivier Bernard, Monique Ras, Jean-Philippe Steyer, Benoît Chachuat</i>	
Design of Continuous Processes for Organic-Synthesis Based Production of Active Pharmaceutical Ingredients — A Methodology	831
<i>Albert E. Cervera, Krist V. Gernaey, Rafiqul Gani, Søren Kiil, Tommy Skovby</i>	
Computational Molecular Design of Drug Delivery Vehicles for Anti-HIV Microbicides	833
<i>Taylor Wilson, Amber Markey, Kyle V. Camarda, Sarah L. Kieweg</i>	
Rapid Interval Arithmetic Screening of Continuous Pharmaceutical Processes with Explicit Thermodynamics	834
<i>Dimitrios I. Gerogiorgis</i>	
Multilevel Control System Integration through An Ontological Chemical Flexible Infrastructure	837
<i>Edrisi Muñoz, Gonzalo Bottaro, Antonio Espuña, Luis Puigjaner</i>	
A Cyber-Infrastructure for Research Collaboration and Knowledge Sharing in the Pharmaceutical Domain: The pharmaHUB	845
<i>José Miguel Laínez, Linas Mockus, Michael J. McLennan, Gintaras V. Reklaitis</i>	
Semantically Enriched High-Throughput Optimization	847
<i>Claudia Labrador-Darder, Antonis Kokossis, Patrick Linke, Franjo Cecelja</i>	

TOPS: Ontological Informatics in Pharmaceutical Manufacturing	849
<i>Girish Joglekar, Arun Giridhar, Gintaras V Reklaitis, Venkat Venkatasubramanian</i>	
MOSAIC: A Web-Based Modeling Environment for Process Systems Engineering	850
<i>Stefan Kuntsche, Harvey Arellano-Garcia, Günter Wozny</i>	
Group Mini Design Projects for Freshman Intro to Engineering	857
<i>Noelle K. Comolli, Randy D. Weinstein</i>	
Integrating Communication Skills and Fostering Collaboration in the Mass and Energy Balances Course with Team Activities	858
<i>Susan Daniel, Kathryn Dimiduk</i>	
Improving Communication Between Sophomores and Juniors through Chem-E-Car Project	859
<i>Sundararan. V. Madihally, Karen A. High</i>	
Teaching the Value of Communication in the Engineering Design Cycle	860
<i>Taryn M. Bayles</i>	
Student Assessment Results of Incorporating Multidisciplinary Industrial Design Problems in the Chemical Engineering Curriculum	861
<i>Jeffrey R. Seay, Jimmy L. Smart, Stephen Hutcherson, David L. Silverstein</i>	
Reality of Remote Experiments in Dynamics and Control from Zacatecas Mexico in the Laboratory of the University of Tennessee at Chattanooga	862
<i>Jose Alberto Gonzales, Jim Henry, Benito Serrano</i>	
Modelling the Internal Resonance Effect in Counter-Current Processes	873
<i>Heinz A. Preisig</i>	
Sustained Oscillations in Continuous Crystallizers	874
<i>Juan Du, B. Erik Ydstie</i>	
Dependence of Film Surface Roughness and Slope On Lattice Size in Thin Film Deposition	875
<i>Jianqiao Huang, Gangshi Hu, Gerassimos Orkoulas, Panagiotis D. Christofides</i>	
Resource-Aware Control of Spatially Distributed Processes Using An Adaptive Predictor-Corrector Strategy	877
<i>Zhiyuan Yao, Nael H. El-Farra</i>	
Model Predictive Control of Czochralski Crystal Growth Process with Time-Varying Spatial Domain	879
<i>James C. Ng, Stevan Dubljevic</i>	
Reduced-Order Control Relevant Model for An On-Board Fuel Processing System	881
<i>M. Sudhakar, Niket S. Kaisare</i>	
Rigorous Convex Enclosures of the Reachable Sets of Nonlinear ODEs Under Uncertainty	883
<i>Joseph K. Scott, Paul I. Barton</i>	
Addressing the Placement of Sensors in IGCC Power Plants through An Efficient Stochastic Mixed Integer Nonlinear Programming Algorithm	885
<i>Adrian J. Lee, Urmila Diwekar</i>	
A Multiparametric Mixed-Integer Quadratic Approximation Algorithm for the Solution of Process Engineering Problems Under Uncertainty	887
<i>Luis F. Dominguez, Efstratios N. Pistikopoulos</i>	
Mixed Integer Linear Programming Formulation of Value at Risk and Conditional Value at Risk for General Stochastic Programs	889
<i>Matthew Colvin, Christos T. Maravelias</i>	
Optimization of Crude Oil Purchasing and Blending Under Uncertainties	891
<i>Yanqin Wen, Jian Zhang, Qiang Xu</i>	
Design Methodology of Modifier-Adaptation RTO Systems	892
<i>Eric Rodger, Benoît Chachuat</i>	
Design and Control of An Energy Integrated Solid Oxide Fuel Cell System	894
<i>Dimitrios Georgis, Sujit S. Jogwar, Ali S. Almansoori, Prodromos Daoutidis</i>	
Energy Storage Technology Selection for Hybrid Fuel Cell Vehicles: A Globally Optimal Control System Based Approach	895
<i>Syed Kaschif Ahmed, Donald J. Chmielewski</i>	
Dynamic Modeling of Thermal Gradients in Solid Oxide Fuel Cells	896
<i>Benjamin J. Spivey, Thomas F. Edgar</i>	
Impacts of Practical Considerations On the Steady-State Behavior of a Solid Oxide Fuel Cell	897
<i>Mona Bavarian, Masoud Soroush</i>	
Minimizing Energy Consumption in Reverse Osmosis Membrane Desalination Using Optimization-Based Control	899
<i>Alex Bartman, Aihua (Richard) Zhu, Panagiotis D. Christofides, Yoram Cohen</i>	
Energy Efficient Model Predictive Control of Buildings	901
<i>Matt Wallace, Prashant Mhaskar, Tim Salisbury, John House</i>	

Optimal Control of Biodiesel Production in a Batch Reactor in the Face of Feed Variability	903
<i>Pahola T. Benavides, Urmila Diwekar</i>	
Centralized Management of Pharmaceutical Clinical Trial Supply Chain	904
<i>Ye Chen, Gintaras V. Reklaitis</i>	
Optimal Energy Supply Network Determination for Hybrid Coal, Biomass, and Natural Gas to Liquid (CBGTL) Plants	906
<i>Josephine A. Elia, Richard Baliban, Xin Xiao, Christodoulos A. Floudas</i>	
Rigorous Decomposition Method for Upstream Natural Gas Supply Chain Network Design and Operation Under Uncertainty	909
<i>Xiang Li, Asgeir Tomasgard, Paul I. Barton</i>	
Improving Supply Chain Performance Using Game Theory, Cooperative MPC and Optimization	911
<i>Kaushik Subramanian, James B. Rawlings, Christos T. Maravelias</i>	
Integrated Production Planning and Scheduling of Multi-Site Batch Plants	913
<i>Nikisha Shah, Marianthi Ierapetritou</i>	
Multicriteria Supply Chain Planning in Oil & Gas Industry: Energy and Environmental Considerations	915
<i>Ivan Ordoñez-S., Diana Franco-C., Sandra Montagut-R., Ariel Uribe-R., Carmen Jimenez-B.</i>	
Process Planning Under Uncertainty with Stochastic Inventory Management:	916
<i>Fengqi You, Ignacio E. Grossmann</i>	
Hierarchical Nonlinear Model Predictive Control of Two Time Scale Systems	918
<i>Michael Baldea, Prodromos Daoutidis, Zoltan K. Nagy</i>	
A Mathematical Theory of Manipulating Suspended Multiple Brownian Particles Simultaneously in a Solution	920
<i>Gautam Kumar, Mayuresh V. Kothare</i>	
A Predictive Control Approach for Processes with Multiscale Objectives	922
<i>Ali Rahnamoun, Antonios Armaou</i>	
Coarse-Grain Modeling of Energetic Materials	924
<i>Sergei Izvekov, Peter W. Chung, Betsy M. Rice</i>	
Multivariable Model Predictive Control of Surface Roughness and Slope in a Thin Film Growth Process	925
<i>Xinyu Zhang, Gangshi Hu, Gerassimos Orkoulas, Panagiotis D. Christofides</i>	
Multi-Scale Modeling and Control of a PEM Fuel Cell	927
<i>Syed Kaschif Ahmed, Donald J. Chmielewski</i>	
Stabilizing the Detached Bridgman Process Via Model-Based, Nonlinear Control	928
<i>Andrew Yeckel, Prodromos Daoutidis, Jeffrey J. Derby</i>	
Industry-Academic-Government Test Bed/Innovation Centers On Smart Process Manufacturing	930
<i>Jim Davis, Thomas F. Edgar</i>	
Collaborative CyberInfrastructure Site for Mixed-Integer Nonlinear Programming	932
<i>Ignacio E. Grossmann, Jon Lee, Pietro Belotti, Lorenz T. Biegler, Pedro Castro, Francois Margot, Juan P. Ruiz, Nikolaos Sahinidis, Andreas Waechter</i>	
An Ontological Knowledge-Based System for Identification of Efficient Chemical Production Routes	934
<i>Ravendra Singh, Krist V. Gernaey, Gani Rafiqul, John M. Woodley</i>	
Process Industry Technicians Adoption of New It-Based Systems	936
<i>Faezeh Karimi</i>	
Advances in Non-Linear Multivariate Latent Variable Regression Using Non-Linear Programming Methods	937
<i>Salvador Garcia-Munoz, Rodrigo López-Negrete De La Fuente, Lorenz T. Biegler</i>	
Oil and Gas Cost Basis Model for Purchased Raw Materials	938
<i>Alex Kalos, Tim Rey</i>	
Integrating Process Databases: Image Analysis in Data Analysis Perspective	939
<i>J. Jay Liu, Seongkyu Yoon</i>	
An Algorithm for the Global Optimization of Unconstrained Parameter Estimation Problems	940
<i>Satyajith Amaran, Nick Sahinidis</i>	
Quantifying Material Structural Component Evolution Using Scattering Data and Mixed-Integer Network Component Analysis	941
<i>Ian Tolle, Lealon L. Martin</i>	
Fuzzy Model Clustering (FMC) Algorithm for Multiple Model Learning	942
<i>Vidyashankar Kuppuraj, Raghunathan Rengaswamy</i>	
Dimension Reduction in Turbulent Combustion Modeling	945
<i>Amir Biglari, James C. Sutherland</i>	
Reactive Scheduling for Ethylene Cracking Furnace System	946
<i>Chuanyu Zhao, Chaowei Liu, Qiang Xu</i>	

Optimizing Design Specification for LNG Receiving Terminal Using Dynamic Simulation	947
<i>Chul-Jin Lee, Youngsub Lim, Chonghun Han</i>	
Recent Advances in Reactive Distillation	948
<i>Philip Lutze, Rafiqul Gani, John M. Woodley, Emmanuel A. Dada</i>	
Energy Saving In Crude Oil Atmospheric Distillation Columns by Modifying Vapour Feed Inlet Tray From Pre-Fractionation Train	949
<i>Mehdi Arjmand, Luis Moreno, Longcheng Liu</i>	
Applying Best Practices in Procedural Operations in a Continuous Process	964
<i>Marcus A. Temant</i>	
Investigation Based On Electric Field to Optimize and Design An Energy-Saving Magnesium Electrolysis Cell	984
<i>Yun Zhao, Ze Sun, Guimin Lu, Jianguo Yu</i>	
Understanding Nanoparticle Diffusion and Exploring Interfacial Nanorheology Using Molecular Dynamics Simulations	986
<i>Yanmei Song, Mingxiang Luo, Lenore L. Dai</i>	
Integration of Umbrella Sampling and Nonlinear Dimensionality Reduction Using Diffusion Maps: Iterative Determination of the "Right" Order Parameters	987
<i>Andrew L. Ferguson, Lilia V. Bravewolf, Athanassios Z. Panagiotopoulos, Pablo G. Debenedetti, Ioannis G. Kevrekidis</i>	
Graphical Processing Unit Acceleration of Coarse Grained Molecular Dynamics Simulations of Surfactant Solutions	989
<i>Benjamin G. Levine, David N. Lebard, Russell Devane, Wataru Shinoda, Axel Kohlmeyer, Michael L. Klein</i>	
Monte Carlo and Density Functional Study of the "Drying" Behavior of Adsorbed Yukawa Fluids On the Repulsive/Attractive Solid Surfaces	990
<i>Lloyd L. Lee, Giuseppe Pellicane, Kevin L. Gering</i>	
Lattice Kinetic Monte Carlo Simulations of Convectively-Driven Particle Aggregation	991
<i>Matthew H. Flamm, Talid Sinno, Scott L. Diamond</i>	
Adsorption Behavior of Homogeneous Model Proteins On Hydrophobic Surfaces From Dissipative Particle Dynamics Simulations	993
<i>Kristin Patterson, Martin Lisal, Coray M. Colina</i>	
Smooth Particle Hydrodynamics of Droplet Formation in Microscale Flows	995
<i>Marion Vance, Kyle D. Squires</i>	
A Graph Theoretic Approach to Time Scale Analysis of Energy Integrated Networks	996
<i>Sujit S. Jogwar, Srinivas Rangarajan, Prodromos Daoutidis</i>	
Networked Control of Nonlinear Spatially Distributed Process Systems	997
<i>Zhiyuan Yao, Nael H. El-Farra</i>	
RNEDE: Resilient Network Design Environment	999
<i>Venkat Venkatasubramanian, Tanu Malik, Arun Giridhar, Kris Villez, Raghendra Prasad, Aviral Shukla, Craig Reiger, Keith Daum, Miles McQueen</i>	
Coarse-Graining the Dynamics of (and on) Networks	1001
<i>Karthikeyan Rajendran, Andreas C. Tsoumanis, Yannis G. Kevrekidis</i>	
Iterative Distributed Model Predictive Control of Nonlinear Systems: Handling Delayed Measurements	1003
<i>Jinfeng Liu, Xianzhong Chen, David Muñoz De La Peña, Panagiotis D. Christofides</i>	
The "Wired" Universe of Organic Chemistry	1005
<i>Siowling Soh, Bartłomiej Kowalczyk, Yanhu Wei, Bilge Baytekin, Chris Gothard, Michal Branicki, Bartosz Grzybowski</i>	
How to Make Use of CAPE-OPEN?	1006
<i>Michel Pons</i>	
ICAS-MoT, a Computer-Aided Modeling Tool	1014
<i>Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani</i>	
Development of An Open Architecture Software Platform for Computer-Aided Design Simulation and Optimization of Polymerization Processes	1016
<i>Apostolos Krallis, Vassilis Saliakas, Costas Kiparissides</i>	
A Hierarchical Modeling Approach to Process Design and Simulation	1018
<i>Robert Kraus, Harvey Arellano-Garcia, Guenter Wozny</i>	
An Equation-Oriented Approach for Handling Thermodynamics Based On Cubic Equation of State in Process Optimization	1019
<i>Ravindra S. Kamath, Ignacio E. Grossmann, Lorenz T. Biegler</i>	
Model Generation for Distributed Systems in Life-Sciences and Biology	1020
<i>Andreas A. Linninger</i>	

The Five Levels of Modelling	1021
<i>Heinz A. Preisig, Tore Haug-Warberg</i>	
CAPE OPEN Interface at BASF	1023
<i>Sergej A. Blagov, Werner Drewitz, Jasper M. Van Baten</i>	
Computer-Aided Emergency Operation of Process Plants	1030
<i>Santos Galán, Laura Lanchas</i>	
Integration of Nonlinear CDU Models in Refinery Planning Optimization	1040
<i>Abdulrahman M. Alattas, Ignacio E. Grossmann, Ignasi Palou-Rivera</i>	
Preventing Thermal Runaway Reaction of Ethylene Oxidation Via Plant-Wide Dynamic Simulation	1043
<i>Xiongtao Yang, Qiang Xu, Kuyen Li</i>	
A Novel Approach to Develop Real-Time Leading Indicators to Predict Incidents in Chemical Plants by Utilizing near-Misses	1045
<i>Ankur Pariyani, Ulku Oktem, Warren D. Seider, Masoud Soroush</i>	
Coordinated Steel Plant Scheduling Solution	1046
<i>Iro Harjunkoski, Sleman Saliba, Matteo Biondi, Chaojun Xu, Guido Sand</i>	
Source Inversion and Response Management in Large-Scale Water Distribution Systems	1047
<i>Angelica V. Wong, Sean McKenna, William Hart, Carl D. Laird</i>	
Consuming CAPE-OPEN Thermodynamics From Multi-Threaded Applications	1049
<i>Jasper M. Van Baten</i>	
Continuous Production in Pharmaceutical Manufacturing: The Informatics View	1058
<i>Arun Giridhar, Girish Joglekar, Gintaras V Reklaitis, Venkat Venkatasubramanian</i>	
Demonstrating the Use of CAPE-OPEN Technology in Process Simulation	1059
<i>Michel Pons</i>	
YODA: A Question- Answering System for Pharmaceutical Informatics	1060
<i>Tanu Malik, Venkat Venkatasubramanian</i>	
Dynamic Optimization with Control Vector Parameterization Using Different Trial Functions: A Comparative Case Study	1062
<i>Nitin Padhiyar, Kartik Shandilya</i>	
An Integrated Fault Diagnosis and Safe-Parking Framework for Fault-Tolerant Control of Nonlinear Process Systems	1070
<i>Miao Du, Prashant Mhaskar</i>	
NLP Sensitivity Based Multi-Rate Moving Horizon Estimation	1074
<i>Rodrigo López-Negrete De La Fuente, Sachin C. Patwardhan, Lorenz T. Biegler</i>	
Model-Based Fault Detection and Fault-Tolerant Control of Process Systems Using Sampled and Delayed Measurements	1076
<i>Yulei Sun, Nael H. El-Farra</i>	
Effect of Soft Sensor Dynamics On Process Monitoring	1078
<i>Mitchell Serpas, Juergen Hahn</i>	
Multivariate Statistical Process Monitoring Based On Statistics Pattern Analysis	1095
<i>Qinghua He, Jin Wang</i>	
Bayesian Fault Detection and Isolation: Test Results for a Simple Benchmark Problem	1097
<i>Kris Villez, Babji Srinivasan, Ulaganathan Nallasivam, Humberto Garcia, Raghunathan Rengaswamy, Shankar Narasimhan, Craig Rieger, Venkat Venkatasubramanian</i>	
Branch and Bound Method for Fault Isolation through Missing Variable Analysis	1102
<i>Vinay Kariwala, Pabara-Ebiere Odiowei, Yi Cao, Tao Chen</i>	
Combining Atomistic and Mesoscopic Simulations to Understand High Shear Dynamics of Chain Molecules	1104
<i>Brian Edwards</i>	
Accelerated Boundary Integral Method in Non-Periodic Geometries	1105
<i>Amit Kumar, Michael D. Graham</i>	
Conditional Quadrature Method of Moments for Kinetic Equations	1106
<i>Cansheng Yuan, Rodney O. Fox, Varun Vikas, Zhijian Wang</i>	
Transport Modeling of Micro- and Nanometer-Sized Particles in a Human Lung Geometry	1107
<i>Erick S. Vasquez, Keisha B. Walters, D. Keith Walters</i>	
The Control and Extinction of Hydrocarbon Flames Via Electric Fields	1109
<i>Kyle J. M. Bishop, Ludovico Cademartiri, George M. Whitesides</i>	
Thermo-Mechanical Modeling of Melt Casting of Explosives	1110
<i>Ruslan S. Mudryy</i>	
Dynamic Unit Operation Model for Industrial Fermentation Processes	1121
<i>Juha Leppävuori, María Soledad Díaz, Lorenz T. Biegler, Michael M. Domach</i>	
A Comprehensive Investigation On Outlier Sources for Models Fitting Experimental Data	1122
<i>Guido Buzzi-Ferraris, Flavio Manenti</i>	

Kinetic Monte Carlo Simulation of Surface Heterogeneity for Lithium-Ion Batteries: Passive Layer Formation and Simulation of Capacity Fade	1136
<i>Ravi N. Methekar, Venkat Subramanian, Kejia Chen, Richard D. Braatz</i>	
Application of Kriging for Dynamic Data-Driven Modeling of Pharmaceutical Processes.....	1139
<i>Fani Boukouvala, Fernando J. Muzzio, Marianthi G. Ierapetritou</i>	
Energy Optimization through Process Integration in Multipurpose Batch Plants: Intermittent Continuous Streams.....	1141
<i>Thokozani Majazi</i>	
Optimal Synthesis of Sequence of CSTR with Non-Linear Cost Objective Function	1142
<i>Paul Ghougassian, Vasilios Manousiouthakis</i>	
Oil Spill Response Planning with Consideration of Oil Transport and Weathering Process: A Multi-Objective Mixed-Integer Dynamic Optimization Approach	1143
<i>Fengqi You, Zhixia Zhong, Sven Leyffer</i>	
Improving the Environmental and Economic Performance of Industrial Processes Using a Multi-Objective Optimization Framework	1146
<i>Nagore Sabio, Carlos Pozo, Gonzalo Guillén-Gosálbez, Laureano Jiménez, Venkatesh Vasudevan, Ramkumar Karuppiah, Nicolas Sawaya, John T. Farrell</i>	
Supervisory Predictive Control of An Integrated Wind/Solar Energy Generation and Water Desalination System: A Two-Time-Scale Approach	1148
<i>Wei Qi, Jinfeng Liu, Panagiotis D. Christofides</i>	
Optimal Pipeline Operations for Unloading Refrigerated Liquefied Petroleum Products.....	1150
<i>Arun Srikanth, Shankar Narasimhan, Sridharakumar Narasimhan</i>	
Optimal Design and Operation of Flexible Energy Polygeneration Systems.....	1152
<i>Yang Chen, Thomas A. Adams II, Paul Barton</i>	
Refinery-Wide Optimization by Using Novel Model Reduction Techniques.....	1153
<i>Vivek Dua, Taoufiq Gueddar</i>	
Plantwide Controller Design for IGCC with Co-Production of Hydrogen and External Steam	1155
<i>Priyadarshi Mahapatra, B. Wayne Bequette</i>	
Data-Based Monitoring and Reconfiguration of Distributed Model Predictive Control Systems	1156
<i>David Chilin, Jinfeng Liu, David Muñoz De La Peña, Panagiotis D. Christofides, James F. Davis</i>	
Design of Optimal Sensor Network Based On Economic Objectives	1158
<i>M. Nabil, Sridharakumar Narasimhan</i>	
Experiences in the Synchronization of Batch Trajectories for Pharmaceutical Process Analysis and Monitoring.....	1160
<i>Salvador Garcia-Munoz, Mark Polizzi, Andrew Prpich, Cathal Strain, Adam Lalonde, Vilmary Negron</i>	
Data-Based Methods for Control of Batch Processes	1161
<i>Siam Aumi, Prashant Mhaskar</i>	
Application of Just-in-Time Statistical Process Control to Vinyl Acetate Monomer Process	1166
<i>Takeaki Sakata, Manabu Kano, Shinji Hasebe</i>	
Diagnosis of Source of Oscillations in Linear Closed-Loop Chemical Processes.....	1178
<i>Babji Srinivasan, Ulaganathan Nallasivam, Raghunathan Rengaswamy</i>	
Detection of Control Loop Interaction and Prioritization of Loop Maintenance.....	1179
<i>M. A. A. Shoukat Choudhury, Anisur Rahman</i>	
A Novel Constrained Total Least Squares Formulation for the Identification of Gene Networks From Highly Noisy and Correlated Measurements.....	1181
<i>Ugur Guner, Matthew Realff, Jay H. Lee</i>	
Design of Constrained Experiments for Identification of Multivariable Fir Models.....	1185
<i>Mark Darby, Michael Nikolaou</i>	
Optimal Experimental Designs Robust to Implementation Errors	1186
<i>Spencer D. Schaber, Paul I. Barton</i>	
Identification for Control of Batch Processes Using Latent Variable Models.....	1187
<i>Masoud Golshan, John Macgregor</i>	
Optimal Parameter Estimation of Stochastic Izhikevich Single Neuron Model Using Experimental Inter-Spike Interval Data.....	1191
<i>Gautam Kumar, Vikram Aggarwal, Nitish V. Thakor, Marc H. Schieber, Mayuresh V. Kothare</i>	
Simplified Dynamic Model of a Solar Thermal Reactor for Biomass Gasification	1193
<i>Elizabeth Saade, David E. Clough, Alan Weimer</i>	
Dynamical Model Reduction Using the Green's Function Matrix.....	1194
<i>Thanneer Malai Perumal, Sai Sandeep Tallam, Rudyanto Gunawan</i>	
Optimal Experimental Design for Isotopic Tracing Experiments of Tumour Metabolism.....	1196
<i>Constantinos Theodoropoulos, Michael Binns, Vitaly Selivanov, Silvia Marin, Marta Cascante</i>	

Computational Strategies for the Global Optimization of Kinetic Models of Metabolic Networks	1198
<i>Carlos Pozo, Gonzalo Guillén-Gosálbez, Laureano Jiménez, Albert Sorribas</i>	
Structure Based Drug Design for Insulin Degrading Enzyme	1200
<i>Seda Kizilel, Ezgi Dagyildiz, Bilal Çakir, Onur Dagliyan, I. Halil Kavakli, Metin Turkay</i>	
Extreme Pathways of Biochemical Reaction Networks Under Thermodynamic Constraints	1206
<i>Vassily Hatzimanikatis, Ho Ki Fung, Keng Cher Soh</i>	
Nonlinear Dynamics and Complexity of the Thyroid Homeostatic Mechanism	1207
<i>Dimitrios I. Gerogiorgis</i>	
Using a Semi-Mechanistic Model of Colorectal Cancer Development to Identify the Sources of and Quantify the Patient and Clinical Costs of Follow-up Colonoscopy Under- and Over-Use	1209
<i>Eric Sherer, Sanmit Ambedkar, Sally Perng, Yuehwern Yih, Tom Imperiale</i>	
Dynamics and Control of Energy Integrated Distillation Column Networks	1211
<i>Sujit S. Jogwar, Prodromos Daoutidis</i>	
Quasi-Decentralized Networked Output Feedback Control of Process Systems Using a Dynamic Communication Policy	1212
<i>Yulei Sun, Nael H. El-Farra</i>	
Multirate Distributed Model Predictive Control of Nonlinear Uncertain Systems	1214
<i>Mohsen Heidarinejad, Jinfeng Liu, David Muñoz De La Peña, James F. Davis, Panagiotis D. Christofides</i>	
A Fault Tolerant Control Framework in Reactor Networks with Agent-Based Systems	1216
<i>Quan Min Shao, Sinem Perk, Ali Cinar, Donald J. Chmielewski</i>	
Safe-Parking of Networked Process Systems with Recycle Streams	1218
<i>Rahul Kumar Gandhi, Prashant Mhaskar</i>	
Reservoir Optimization with Model Parameter Uncertainty Updates	1220
<i>Yingying Chen, Karlene Hoo</i>	
Novel Block Decentralized MPC Control for Local Autonomy	1223
<i>Thomas E. Marlin, Alberto Jorge Olvera</i>	
Author Index	