TABLE OF CONTENTS

Volume 1

Opening Remarks................................................................................................................................. 1
   Francis J. Doyle III

Computation in Undergraduate ChEmical Engineering Education .................................................. 2
   Bruce A. Finlayson

Smart Process Manufacturing – Results from An NSF-Sponsored Workshop.................................... 25
   Thomas F. Edgar, Jim Davis

Integration of Computational Fluid Dynamics (CFD) into the ChEmical Engineering Undergraduate Curriculum ................................................. 26
   Richard D. Luscombe

The Cache Systems Biology Task Force.............................................................................................. 27
   Michael H. Henson

Molecular Modeling Task Force Update .............................................................................................. 28
   David A. Kofke

Cache Modules on Energy in the Curriculum: Fuel Cells.................................................................... 29
   Jason M. Keith, Michael D. Gross, Donald J. Chmielewski, H. Scott Fogler

Current Attributes and Future Prospects for Polymath Software .................................................... 30
   Michael B. Cutlip, Mordechai Shacham

Education Modules in Process Design and Operability ........................................................................ 31
   Thomas E. Martin

Model-Based Innovations In Process Development and Design........................................................ 33
   Constantinos C. Pantelides

Advances in Process Synthesis - Energy & Environment .................................................................... 34
   Robin Smith

Process Synthesis of Separation Systems .......................................................................................... 36
   Manfred Morari

In the Spirit of Carnot: Theoretical Limits to Steady-State Productivity .......................................... 37
   Yangzhong Tang, Philipp Ellison, Martin Feinberg

One History of Industrial Process Synthesis ..................................................................................... 38
   Jeffrey J. Sühring

In Honor of the 60th Birthday of George Stephanopolus .................................................................... 39
   Gregory N. Stephanopoulos

Process Dynamics and Control .......................................................................................................... 40
   Manfred Morari

Process Synthesis and Optimization .................................................................................................... 41
   Ignacio E. Grossmann

Biomolecular Separations and Downstream Processing ...................................................................... 42
   Georges Belfort

Thermodynamics and Statistical Mechanics ....................................................................................... 43
   Pablo G. Debenedetti

High Throughput Heterogeneous Catalyst Research .......................................................................... 44
   Henry Weinberg

Process Operations for Batch and Continuous Processes ................................................................... 45
   G. V. Reklaitis

Opportunities for Process Development in the Conversion of Biomass to Fuels and ChEmicals .......... 46
   James A. Dumesic

Systems Biology: An Era of Reconstruction and Interrogation ......................................................... 47
   Bernhard O. Palsson

Creating Technologies for New Businesses: Insights on Innovation ................................................. 48
   Gary Calabrese

Graphics Processing Units for High-Performance Computing in Bioinformatics .................................. 49
   Panagiotis Fountis, Joe Elble, Nick Sahinidis

Fully-Implicit Finite Element Formulations for Stability and Bifurcation Analysis of Large-Scale Resistive
Magneto-Hydrodynamic Systems ......................................................................................................... 50
   Roger P. Pawlowski, John N. Shadid
Model Reduction-Based Constrained Optimisation for Large-Scale Steady State Systems Using Black-Box Simulators ......................................................................................................................................................................................................51
Ioannis Bonis, Constantinos Theodoropoulos

Canonical Primal-Dual (CPD) Formulation of Process Models ......................................................................................................................................................................................................59
Cliff Amundsen, Ross Swaney

Hybrid Niche Algorithm for Problem Inversion of Distributed Systems with Solution Multiplicity .................................................................61
Jeonghwa Moon, Libin Zhang, Andreas A. Linnenger

Taylor Based Pseudo-Analytical Solution of the Power Law Model for Non-Newtonian Fluid In FREE Convective Cells .................................................................62
Mario Oyanader, Pedro E. Arce

A New Efficient Eigenvalue Bounding Method for Convexity Detection with Applications in Global Optimization and Control ......................................................................................................................................................................................................63
Martin Mönnigmann

Computational Comparison of Piecewise Linearization Schemes in Gas Lifting and Pooling Optimization Problems ......................................................................................................................................................................................................67
Ruth Misener, Chrysanthos E. Gounaris, Christodoulos A. Floudas

Global Solution of Bilevel Mixed-Integer Nonlinear Programs ......................................................................................................................................................................................................69
Alexander Mitsos

Global Optimization of Mixed-Integer Bi-Level Programming Problems Via Multi-Parametric Programming .................................................................71
Luis F. Dominguez, Efstratios N. Pistikopoulos

Relaxations of Nonconvex, Quadratically-Constrained Quadratic Programs ......................................................................................................................................................................................................72
Xiaowei Bao, Nick Sahinidis

Polyhedral Results for a Discrete-Time Mip Formulation for Production Planning ......................................................................................................................................................................................................73
Christos T. Maravelias

A Kriging Optimization Algorithm Incorporating Efficient Sampling for Problems Containing Black-Box Models .................................................................75
Eddie Davis, Marianneh Ierapetritou

Distributed Optimization and Control of Offshore Oil Production: The Intelligent Platform .................................................................78
Michael R. Wartmann, B. Erik Ydstie

Cogeneration Power Plant Operation: A Novel Controller Assessment Method for Improving Disturbance Rejection Performance ......................................................................................................................................................................................................79
Rachelle Howard, Douglas Cooper

Optimal Scheduling with Energy Constraints ......................................................................................................................................................................................................82
Pedro Castro, Ilro Harjunkoski, Ignacio E. Grossmann

Integrated Hedging and Operations for Complex Energy Utilities ......................................................................................................................................................................................................83
Jeffrey Kantor, Anees Attarwala, Patrick Mousaw

Life Cycle Assessment Coupled with Multi-Objective Optimization for Environmentally Conscious Planning of Energy Production Systems ......................................................................................................................................................................................................85
Gonzalo Guillén-Gosálbez, Metin Turkay

Simplification of the Inviscid Navier-Stokes Equations for Dynamic Simulation of Nonisothermal Gas Flow Networks ......................................................................................................................................................................................................87
Patricia D. Ramirez-Manoz, Majid S. Kazimi, Paul I. Barton

Classification of ChEmical Processes. A Graphical Approach Using Heat Engine Concept ......................................................................................................................................................................................................89
David Glasser, Diane Hildebrandt

Design Heuristics for Semicontinuous Separations with Reaction ......................................................................................................................................................................................................90
Thomas A. Adams II, Warren D. Seider

Translation of Variables for Different Applications in Process Synthesis ..................................................................................................................................................................................................................92
Marcel Rapotar, Zdranko Kravanja

A Bilevel Framework for Process Design & Operation ......................................................................................................................................................................................................100
Alexander Mitsos, Panayiotis Lemonidis, George M. Bollas, Benoit Chachuat, Paul I. Barton

A Novel Approach for Global Optimization of Stage-Wise Heat Exchanger Network Models ......................................................................................................................................................................................................103
Miguel J. Bagajewicz, Milos Bogatay, Debora C. Faria

Minimum Capital and Minimum Total Annualized Cost for a Power Plant Using the Ideas Framework ......................................................................................................................................................................................................104
Jorge Pena Lopez, Vasilios I. Manousiouthakis

A Metric for Monitoring Mpc Optimization Strategy ......................................................................................................................................................................................................105
William Canney

Computation of Arrival Cost for Moving Horizon Estimation Via Unscented Kalman Filtering ......................................................................................................................................................................................................106
Cheryl C. Y. Qu, Juergen Hahn

Nonlinear Stochastic Modeling for State Estimation of An Industrial Polymerization Process ......................................................................................................................................................................................................117
Fernando V. Lima, James B. Rawlings, Tyler A. Soderstrom

Design of Experiments for Identification of Multivariable Models Satisfying Integral Controllability: The Dynamic Model Case ......................................................................................................................................................................................................119
Mark Darby, Michael Nikolau
A Systematic Bi-Level Approach for Efficient Process Optimization Under Uncertainty Using Stochastic Annealing .............................................................. 385
Aparnasia J. Papadopoulos, Panos Seferlis

L-Shaped Bonus Algorithm with Application to Water Pollutant Trading .................................................. 387
Yegendra Shastri, Urmila Diversekar

Distributed Control System Design Using Lyapunov-Based Model Predictive Control .................................. 388
Panagiotis D. Christofides, David Muñoz De La Peña, Jinfeng Liu

A Parallel Algorithm for Efficient Large-Scale Dynamic Optimization ......................................................... 389
Arndt Hartwich, Wolfgang Marquardt

Quasi-Decentralized State Estimation and Output Feedback Control of Process Systems Over Communication Networks ........................................................................... 398

Cooperative, Distributed Model Predictive Control for Systems with Coupled Input Constraints .................. 400
Brett Stewart, James B. Rawlings

Large-Scale Optimization Strategies for the Operation of Low-Density Polyethylene Tubular Reactors ........ 402
Victor M. Zavala, Lorenz T. Biegler

Analytical Results for Tiered Intermediate Product Prices for Apc Using a Refinery Lp .............................. 403
Jeyarathan Arjunan, James R. Whiteley

Implementation of Coordinator Mpc on a Large-Scale Gas Plant .............................................................. 405
Elvira M. B. Aske, Stig Strand, Sigurd Skogestad

Cyberinfrastructure (CI) Funding In the Engineering Directorate (ENG) of the National Science Foundation (NSF) .......................................................................................................................... 409
Maria K. Burk

Pharmaceutical Informatics and New Financial Models of the Bio-Pharma Industry ......................................... 410
Sangtae Kim

Challenges in Biological Informatics ............................................................................................................... 411
Nick Sahinides

Semantic Workflow and Information Management in Process Engineering .............................................. 412
Wolfgang Marquardt

Informatics Needs, Challenges and Opportunities in ChEmical Engineering: Roundtable Panel Discussion ........................................................................................................................................ 418
Larry Megan, Venkat Venkatasubramanian

Model-Based Product and Process Development for Polymers in An Industrial Environment .................. 419
Klaus-Dieter Hungenberg

Development of on-Line Optimization-Based Control Strategies for a Starved-Feed Semi-Batch Copolymerization Reactor ........................................................................................................... 420
Onyinye E. Okoroafo, Luis Fernando Torres, Robin A Hutchinson, Martin Guay

Determination of the Dominant Nucleation Mechanism for Oil-Soluble Initiators In Miniemulsion Polymerization Using Kinetic Monte Carlo Simulations ......................................................................... 429
Jonathan A. Rawlston, Juchen Gao, F. Joseph Schork, Martha Grover Gallivan

Modular Optimization and Optimal Control of Polymerization Reactions .................................................. 431
Michael Wulkow

Zheng Liu, Yinlun Huang, Zhen Wu

Experiences in the Building of Dynamic Flowsheet Models for Embedded Nonlinear Control .................... 437
Kenneth V. Allsford, John Goodman, Jeffrey G. Kenfro

Advanced Process Control for ChEMical Batch Reactors Applied to a Polymerization Process .................. 444
Wim Van Brempth

Electromechanically-Driven Complex Void Dynamics In Metallic Thin Films ................................................ 451
Vivek Tomar, M. Rauf Gangor, Dimitrios Maroudas

Elastic Stability and Structural Response of Body-Centered Cubic Crystals Under Uniaxial and Hydrostatic Loading ................................................................................................................... 453
Hadrian Djohari, Frederick Milstein, Dimitrios Maroudas

Engineering Complexity In ChEmically-Reacting Dynamical Systems: Studies on Electrode Arrays ............. 454
Craig G. Rusin, Irvan Z. Kiss, Hiroshi Kori, John L. Hudson

Dynamical Behaviour of the Phenylacetylene Carbonation Reaction in a Calorimeter ................................. 455
Ankur Mukherjee, Katarina Novakovic, Dominic P. Searson, Mark Willis

Effect of Gas-Liquid Mass Transfer Rates on the Palladium Catalysed Phenylacetylene Oxidative Carbonylation Reaction ............................................................................................................. N/A
Katarina Novakovic, Mark J. Willis, Allen R. Wright

Front Velocity and Criterion of Transversal Patterns In Packed-Bed Reactors ........................................... 456
Moshe Sheintuch, Olga Nekhamkina
<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pattern Formation and Chaotic Dynamics In a Model of Simultaneous Oxidation and Reduction In Three-Way</td>
<td>458</td>
</tr>
<tr>
<td>Catalytic Converters</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>A Statistics Pattern Based Framwork for Process Monitoring</td>
<td>459</td>
</tr>
<tr>
<td>Qionghua (Peter) He, Jin Wang</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Agent-Based Distributed Monitoring and Fault Detection</td>
<td>461</td>
</tr>
<tr>
<td>Sinem Perk, Fouad Teymour, Ali Cinar</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Real-Time Kinetic Hard-Modelling for the Optimisation of Reaction Conditions and the Detection of Process</td>
<td>463</td>
</tr>
<tr>
<td>Upset in Semi-Batch Reactors</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Industrial Implementation of on-line Multivariate Quality Control (Part III: Relationship to molecular weights)</td>
<td>465</td>
</tr>
<tr>
<td>Le H. Chiang, Kathy Walsh, Shawn Maynard, Bart Neff, Lloyd Colegrove</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Dempster-Shafer Fusion for Collaborative Fault Detection and Identification (FDI) with Application to a</td>
<td>N/A</td>
</tr>
<tr>
<td>Distillation Column Case Study</td>
<td></td>
</tr>
<tr>
<td>Kaushik Ghosh, Yew Seng Ng, Rajagopalan Srinivasan</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Fault-Detection and Isolation and Fault-Tolerant Control of Nonlinear Process Systems Using Asynchronous</td>
<td>466</td>
</tr>
<tr>
<td>Measurements</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Fault Tolerant Controller Design for Transport-Reaction Processes Employing Spatial Controllability</td>
<td>467</td>
</tr>
<tr>
<td>Antonios Armou, Michael A. Demetriou</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Centralized - Decentralized Optimization for Refined Rerouting</td>
<td>468</td>
</tr>
<tr>
<td>Nikisha Shah, Zhenya Jia, Georgios Saburides, M. G. Ierapetritou</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Dynamic Modeling of a Global Specialty Chemicals Supply Chain</td>
<td>470</td>
</tr>
<tr>
<td>Charles Wei Kang Wong, Arief Adhitya, Rajagopalan Srinivasan</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimization of Discrete Time Supply Chain Models with Guaranteed Robust Stability and Feasibility</td>
<td>471</td>
</tr>
<tr>
<td>Darya Kastsi, Martin Mönigmann</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>A Process Attainable Region Approach for Supply Chain Management</td>
<td>477</td>
</tr>
<tr>
<td>Charles Sung, Christos T. Maravelias</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Selection of Third-Party Service Contracts for ChEmical Logistics</td>
<td>479</td>
</tr>
<tr>
<td>Muka Bansal, I. A. Karimi, Raj Srinivasan</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Optimal Supply Chain Design with Multi-Echelon Stochastic Inventory and Risk-Pooling</td>
<td>481</td>
</tr>
<tr>
<td>Fengyi You, Ignacio E. Grossmann</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Design of An on-Farm Ethanol Dewatering System</td>
<td>483</td>
</tr>
<tr>
<td>Anuradha Mukherjee, James R. Whiteley, Danielle Bellmer</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>A Process Integration Approach to Strategic Design and Scheduling of Multi-Feedstock Biodiesel Plants</td>
<td>485</td>
</tr>
<tr>
<td>René D. Elms, Grace Nvorie, Mahmoud M. El-Halwagi</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Online State Estimation In Enzymatic Synthesis of Ampicillin Process: Experimental and Simulation Study</td>
<td>486</td>
</tr>
<tr>
<td>Marcelo Ferencin De Arruda Ribeiro, Roberto De Campos Giordano, Sridhar Ungarala</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-Linear Parameter Estimation for a Dynamic Model of Mammalian Cell Culture</td>
<td>489</td>
</tr>
<tr>
<td>Adam C. Baughman, Susan Sharfstein, Lealon L. Martin</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Decision-Making In Biopharmaceutical Process Design</td>
<td>490</td>
</tr>
<tr>
<td>Charles Siletti, Demetri Petrides</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Formulation of a Herbal Medicinal Product - Sheng Mai San</td>
<td>491</td>
</tr>
<tr>
<td>Elizabeth J. Zhang, Kam M. Ko, Ka M. Ng</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>A Framework for Assessing the Biocomplexity of Sustainable Material Use</td>
<td>492</td>
</tr>
<tr>
<td>Jun-Ki Choi, Bhavik R. Bakshi, Timothy C. Haub, Prem K. Goel</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Safeparking of Multi-Unit Process Systems</td>
<td>494</td>
</tr>
<tr>
<td>Rahul Gandhi, Prashant Bhaskar</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Model-Based Sensor Scheduling for Power Management In Wireless Sensor Networks</td>
<td>496</td>
</tr>
<tr>
<td>Yules Sun, Nael H. El-Farra</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Modeling Technology Transitions and Risks Using Input-Output Framework</td>
<td>499</td>
</tr>
<tr>
<td>Vikas Khanna, Bhumik B. Bakshi</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>A Reaction Route Network Approach to the Thermodynamic Consistency of Microkinetic Models</td>
<td>501</td>
</tr>
<tr>
<td>Michael Morin, Saurabh Véckal, Ravi Dutta, Ilie Fishtik</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Graph-Theoretic Approach for Discovering Alternative Synthetic Routes Forming Complex Networks</td>
<td>502</td>
</tr>
<tr>
<td>L. T. Fan, Tengyan Zhang, A. Argosti, Jiachong Liu, Botond Bertok, Ferenc Friedler</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Integrating Networked Process Systems to Solve Dynamic Optimization Problems</td>
<td>503</td>
</tr>
<tr>
<td>B. Erik Ydstie, Michael R. Wartmann</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Explicit Real-Time Optimization</td>
<td>504</td>
</tr>
<tr>
<td>Johannes E. P. Jäschke, Srihararukumar Narasimon, Sigurd Skegestad</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Identification and Control of a Tubular Solid Oxide Fuel Cell (SOFC)</td>
<td>506</td>
</tr>
<tr>
<td>Debangsu Bhattacharyya, Rahulnathan Rengaswamy, Finnerty Caine</td>
<td></td>
</tr>
</tbody>
</table>
Passivity Based Modeling and Control of Coal Power Plants ................................................................. 507
B. Erik Yatsire, Chengtao Wen

Cfd Simulation of Urea-Based Hybrid Sncr-Scr in a Pilot Scale Flow Reactor ................................................. 509
Thanh D. B. Nguyen, Tae-Ho Kang, Young Il Lim, Seong-Joon Kim, Kyung-Seon Yoo

Fast Nonlinear Predictive Control of Autothermal Hydrogen Generation Subject to Economic Constraints ........ 510
Michael Baldea, Prodromos Daoutidis, Zofia K. Nagy

Stochastic Prediction and Control of Cyclic Combustion Variation in Internal Combustion Engines .................. 512
James C. Peyton Jones, Kenneth R. Muske

Estimation of Spatial Coupling and Temporal Dynamics In the Spread of Childhood Infectious Disease .............. 513
Carl D. Laird, Derek A. Cummings, James Young

Verified Solution of Epidemiological Models with Probabilistic Uncertainty ..................................................... 515
Joshua A. Enzner, Mark A. Stadtherr

Estimation of Infectious Disease Parameters from Initial-Time Asymptotic Analysis ............................................ 516
Kenneth R. Muske, Hashem Ashrafiuon, Alan M. Whitman

Engineering Control Approaches for the Design and Analysis of Adaptive Behavioral Interventions .................. 519
Daniel E. Rivera, Linda M. Collins

Modeling the Control of An Excitatory Neurotransmitter Receptor during Alcoholism and Alcohol Withdrawal .......... 520
Mary K. McDonald, James S. Schwaber, Babatunde A. Ogunnaike

Blood Glucose Regulation with An Adaptive Model-Based Control Algorithm .................................................. 522
Merijan Eren-Oruklu, Ali Cinar, Lauretta Quinn, Don Smith

Human-Friendly and Control-Relevant Modeling for a Closed-Loop Artificial Pancreas ........................................ 524
Hyunjin Lee, B. Wayne Bequette

A New Methodology for Integrated Planning and Scheduling Using Multi-Level Optimization ................................ 527
Zakui Li, M. G. Ierapetritou

Integrated Operational Planning and Medium-Term Scheduling of a Large-Scale Industrial Batch Plant Under Uncertainty .......................................................................................................................... 530
Peter M. Ferdeman, Christodoulos A. Floudas

Bi-Level Planning for Profit Increment In Petroleum Industry .............................................................................. 532
Jian Zhang, Qiang Xu

Cutting Planes and Decomposition Techniques for Solving Large-Scale Milp Model for Petroleum Supply Operations .................................................................................................................................................. 533
Roger Rocha, Ignacio E. Grossmann, Marcia V. S. Poggi De Araujo

Simultaneous Batching and Scheduling In Multi-Stage Processes with Storage Constraints .................................. 535
Aral Sundaramoorthy, Christos T. Maravelias

Refinery Planning Considering Financial Risk Management Using Crude Oil Derivatives ...................................... 536
Jeongho Park, Sunwon Park, Young Kim, Choamun Yun

Enterprise-Wide Data Management Connects People ........................................................................................ 537
Gregory M. Banik

Rapid, Global Communication of Company Policies and Standards ........................................................................ 538
Jeremiah P. Obrien, Richard Wanzel

Net-Centric Integration of Manufacturing, Supply Chain, and Enterprise Management – Delivering the Process Industry’s Equivalent to Sensor Fusion and the Battlefield of Tomorrow ................................................................................................................ 548
Michael R. Basila

Achieving Energy Reductions Via a Global Energy Management System ............................................................... 549
Flynn M. Collins

Roundtable Discussion - Implementing Information Technology Applications to Support Global Organizations ........... 550
Gary K. Stenerson

Volume 2

A Modified Network Component Analysis (NCA) Methodology for the Decomposition of X-Ray Scattering Signatures from Polymers ........................................................................................................... 551
Ian Tolle, Yvonne A. Akpalu, Lealon L. Martin

Multi-Scale Modelling of Chinese Hamster Ovary Cell Cultures ........................................................................... 552
Srinivas Karra, M. Nazmul Karim

A Systematic Multiscale Modelling Framework for Product-Process Design and Development ........................... 553
Ricardo Morales-Rodriguez, Rafiqul Gani

Ab Initio Crystal Structure Determination Using Global Optimization ................................................................. 554
Angelo Lucia, Rajeswar R. Gattupalli

Processmodeller. A Modelling Environment for Multi-Scale, Large-Scale Modelling ............................................ 555
Heinz Preisig
Parameter Set Selection Via Clustering of Parameters into Pair-Wise Indistinguishable Groups of Parameters ......................................................... 557
Yunfei Chu, Juergen Hahn

Construction of Stochastic Differential Equation Models for Porous Thin Film Deposition Processes ......................................................... 568
Gangshi Hu, Xinyu Zhang, Gerasimouss Orkoudis, Panagiotis D. Christofides

Optimal Operation with Respect to Multiscale Objectives during Layered Heterostructure Growth ............................................................... 570
Christopher Behrens, Antonios Arnaout

Multiscale Model Development for Microstructure-Based Product Quality Control In Polymetric Coating Curing ................................................. 572
Jie Xiao, Yinan Huang

Efficient and Robust Multi-Scale Models of Conjugate Heat Transfer and Melt Crystal Growth ................................................................. 573
Andrew Veckel, Lisa Kun, Thomas Jung, Jochen Friedrich, Jeffrey J. Derby

Computational Studies of Semiconductor Nanocrystal Synthesis In Templating Media .................................................................................. 574
Sreekumar Kuriyedath, Yannis G. Kevrekidis, T. J. Mountziazis

Multi-Scale Modelling and Design of Catalytic Microreactor Systems .............................................................................................................. 575
Bostjan Hari, Constantin Theodoropoulos

Temperature Accelerated Dynamics Based Kinetic Monte Carlo Method ........................................................................................................ 576
Abhijit Chatterjee, Blass P. Uberuaga, Arthur F. Voter

Optimal Scheduling of Multistage Batch Plants. A Comparative Study .............................................................................................................. 577
Pedro Castro, Augusto Q. Novais

CP-Based Symmetry-Breaking Branching for Crude-Oil Operations Scheduling .............................................................................................. 579
Sylvain Mouret

A Convex Hull Discretization Approach to the Global Optimization of Pooling Problems ................................................................................. 581
Viet Pham, Carl D. Laird, Mahmoud El-Halwagi

The Unit-Specific General Precedence Scheduling Model: Addressing Sequence-Dependent Setup Times and Costs Issues .................................................. 582
Georgios Kaponos, Luis Puigjaner

A New Network-Based Representation for Process Scheduling ................................................................................................................................. 584
Diego M. Giménez, Gabriela P. Henning, Christos T. Maravelias

Short-Term Scheduling of Multipurpose Batch Processes Using Unit Slots ........................................................................................................ 586
Nareesh Sasara, Jie Li, Karimi I. A.

Fermentative Poly(3-hydroxybutyrate) Production In Alcaligenes Latus: A Combined Metabolic/kinetic Modelling Approach ........................................ 588
Giannis Penelis, Arvandous Roukou, Christos Chatzidounas, Costas Kiparisides

Indirect Response Model of Arsenic Exposure on Gene Expression ...................................................................................................................... 591
Meric Ovacik, M. G. Jerepapetrou, P. G. Georgopoulos, W. Welch, L. P. Androulakis

Design and Optimization of An RNAI Based Biomolecular Logic Circuit ........................................................................................................ 593
Leonidas Bleris, Keller Rinaudo, Rohan Maddamsetti, Sairam Subramanian, Ron Weiss, Yaakov Benenson

Analysis Procedure for Signal Transduction Pathways by Clustering Parameters According to Their Sensitivity Profiles ............................................. 595
Yunfei Chu, Zuyi (Jacky) Huang, Juergen Hahn

The Effect of Biological Variability on the Angiotensin II Gene Regulatory Network In the Central Regulation of Blood Pressure .................................................. 607
Gregory M. Miller, Rajanikanth Vadigepalli, James S. Schwabe, Babatunde A. Ogunnaiske

Optimal Cancer Treatment Using Radiotherapy .............................................................................................................................................. 608
Ricardo Dunita, Thomas Edsion

Combined Statistical and Genom-e-Scale Analysis of Mammalian Cell Lines Producing Bio-Therapeutics ......................................................... 609
Suresh Selvarasu, Dong-Tap Lee, I. A. Karimi

Direct PID Tuning from Closed-Loop Data and Its Application to Unstable Polymerization Process ................................................................. 611
Kenichi Tasaka, Manabu Kano, Motomasa Ogawa, Shiro Matuda, Toru Yamamoto

Inverse Model of the Glass pH Sensor ............................................................................................................................................................... 612
Jietae Lee, Su Whan Song, Scungjae Lee, Daeyook Yang

A Dynamic Systems Approach to the Synthesis and Analysis of Mammalian Metabolic Networks ........................................................................... 616
Adam C. Baughman, Lealon L. Martin, Susan T. Sharfstein

Alternative Model Structure with Simplistic Noise Modelling for Linear Processes Subjected to Non-Stationary Disturbances ........................................ 617
Srinivas Karra, M. Nazmul Karim

Richard W. Bonner III

Multi-Scale Analysis and Control Structure Design for Biotechnological Processes .......................................................................................... 626
Jobrun Nandong, Yudi Samyudia, Moses O. Tade

Robust Nonlinear Model Predictive Control Of An Augmented-Reality Lab-Scale Plant .................................................................................. 640
Udo Schubert, Harvey Arellano-Garcia, Guenter Wozny

Relay with a Negative Hysteresis for Autotuning of Control Systems Under Noisy Environments ........................................................................... 641
Jietae Lee, Su Whan Song, Thomas F. Edgar
Dynamic Optimization of Mma and Vac Copolymerization Process ........................................... 642
Naidoon M. N. Lima, Lamia Zuiliga Lilian, Rabens Maciel Filho, Flavio Manenti, Davide Manca, Marcelo Embiruçu

Modeling and Control of a Packed Distillation Column ................................................................. 643
Carolina Ramírez, Ivan Darío Gu El Chaves, Nicanor Quijano

Challenges to Using Mechanisms of Action to Quantify Efficacy of Nucleoside-Analogue Reverse Transcriptase Inhibitors ........................................................................................................... 645
James Monaco, Samira Khalili, Antonios Armaou

Mpc-Based Integrated Product and Process Control ........................................................................ 646
Zhen Wu, Zheng Liu, Yinlun Huang, Yu Qian

Development of Nonlinear Predictive Model-Based Feedforward Control Framework from Closed-Loop Freely-Existing Real Data .................................................................................................................... 647
Derrick Bollins, Stephanie Loveland, Nidhi Bhandari

Blood Glucose Regulation with Stochastic Optimal Control for Insulin-Dependent Diabetic Patients ...................................................................................................................... 652
Saadat Ulas Akıkgöz, Urmila Dwekar

Data Analysis and Parameter Estimation of Bioprocesses .................................................................. 656
Harvey Arellano-Garcia

Population-Based Colorectal Cancer Care Control ........................................................................... 657
Selén Aydogan-Cremaschi, Tapas K. Das, Chaithra Gopalappa, Seza Orcun

The Physical Structure of Intracellular Feedback Loops ...................................................................... 660
Christopher V. Rao

Assigning Physical Significance to the Diffuse Interface Between Terraces In Phase-Field Modeling of Steps on Crystal Surfaces ........................................................................................................... 661
Igal G. Rasin, Simon Brandon

Catalytic-Pathway Identification for Methanol Decomposition on Pt (1 1 1) Via the Graph-Theoretic Method Based on P-Graphs ........................................................................................................... 662
Yu-Chuan Lin, L. T. Fan, Shahram R. Shafie, Botond Bertok, Ferenc Friedler

Coarse-Grained Kinetic Monte Carlo Models: Complex Lattices, Multicomponent Systems, and Homogenization at the Stochastic Level ...................................................................................... 663
Stuart D. Collins, Abhijit Chatterjee, Dion Vlachos

A Three-Dimensional Interfacial Spectral Boundary Element Algorithm for Capsules and Erythrocytes in Strong Flows ................................................................................................................... 664
Walter R. Dodson III, Panagiotis Dimitrakopoulos

A Software Tool for Design of Process Monitoring and Analysis Systems ........................................... 665
Ravendra Singh, Kris V. Gernaey, Rafiqul Gani

Data-Based Fault Detection and Isolation Using Feedback Control: Output Feedback, Optimality and Asynchronous Measurements ........................................................................................................... 666
Panagiotis D. Christofides, Ben Ohran, David Muñoz De La Peña, James F. Davis

Novel Method for Global Optimization of Nonconvex Minlp Problems ........................................... 668
Debora C. Faria, Miguel J. Bajegiewicz

A Nearest in Control Neighbour Based Method to Estimate Variable Contributions to the Hotelling’s Statistic ............................................................................................................................... 669
Carlos R. Alvarez, Adriana Brandolin, Mabel C. Sanchez, Luis Puigjaner

A Functional Approach to Optimization of Supply Chain Networks with Both Efficiency and Robustness Objectives ......................................................................................................................... 680
Avisrul Shukla, Vishal Agarwal, Venkat Venkatasubramanian

Minimization Under Uncertainty of Fresh Water Consumption for Pulverized Carbon (PC) and Integrated Gasification Combined-Cycle (IGCC) Power Plants ......................................................... 682
Juan M. Salazar, Urmila Dwekar

Enhancing Supply Chain Network Design by Considering Financial Analysis Issues ................................ 683
Georgios Kopanos, José Miguel Laínez, Mariana Badell, Luis Puigjaner

Global Optimization of Noisy Black Box Functions Using the Artificial ChEmical Process and Evolutionary Algorithms ......................................................................................................................... 685
Roberto Irizarry

A Novel Continuous-Time Formulation for Short-Term Scheduling of Continuous Processes ................ 686
Jie Li, Naresh Susarla, I. A. Karimi

Eliminating Gaps Between Advanced Planning and Scheduling Models ............................................... 688
Yanpin Wen, Qing Xu

Building a High-Fidelity Dynamic Simulation and Control System Fast .............................................. 689
David C. Zhou

Identification of the Attainable Region for Batch Reactor Networks ..................................................... 697
Benjamin J. Davis, Vasilios I. Manoussiotakis

Wastewater Treatment: New Perspectives Provided by Interactive Multiobjective Optimization ............. 698
Jussi Hakamies, Kaisa Miettinen, Kristian Sahlinstd
Dynamic Simulation for Best Performance of Multi-Stage Compression System during Plant Startup
Xiongtao Yang, Kuyen Li, Quang Xu .......................................................... 700

Production Planning, Scheduling, and Debottlenecking Practices in the Biopharmaceutical Industries
Charles Siletti, Demetrio Petrides ........................................................... 701

Monitoring, Detection and Diagnosis of Leaks from Gas Pipes Based on Real-Time Data Collected Over the Ubiquitous Sensor Network
Dongil Peter Shin, Jae Wook Ko ............................................................... 702

Energy Optimization through Non-Linear Modeling and Control of Fuel Gas Process at Hovensa
Manish Misra, Victor M. Marrero, Kevin S. Brooks, Hannes De Beer ............... 704

Environmental Evaluation of Cogeneration Scenarios in Sugar Industry
Mauricio Colombo, Fernando Daniel Mele, Maria Rosa Hernandez, Jorge E. Gatica, José Luz Silveira Sr. .............................................................................................................................................................................................. 705

Industrial Biosystems Engineering: Application of Systems Engineering in Biorefinery Systems
Shulin Chen .................................................................................................. 707

Model-Based Fault Detection and Monitoring of Uncertain Hybrid Process Systems
Nael H. El-Farra ........................................................................................... 711

A C.F.D.-Guided Mixed Integer Nonlinear Programming (MINLP) Model for Conceptual Design of a Carbothermic Aluminum Reactor
Dimitrios I. Gergouriatis ............................................................................. 715

Effectiveness of Coatings to Reduce Fouling in Shell and Tube Heat Exchangers
Gabriel T. Fernandez, Talea A. Rothan ......................................................... 716

Cfd Predictions of Bod Removal in Wastewater Treatment Lagoons
Benson Wu ................................................................................................... 717

Heat Integrated Reactive Distillation Designs for Hydrolysis of Methyl Acetate
Hao-Yeh Lee, Hsiu-Ping Huang, Yi-Chen Lee ............................................... 718

Modeling and Simulation of a Pilot-Scale Fixed Bed Reactor for Dimethyl Ether (DME) Synthesis
Dae-Sung Song, Dongil Shin, Wonjun Cho, Dal Keun Park, Eun Sup Yoon ............ 719

Energy Analysis of Chemical Batch Plant through Advanced Integration of Energy Conversion, Production Processes and Waste Management
Claude Retat, Stavros Papadokonstantakis, Konrad Hungerbühler ................. 726

Superstructure-Based Nlp Formulation for Design of Batch Water Networks
Cheng-Liang Chen, Chia-Yuan Chang, Jui-Yuan Lee, Ying-Jyuau Ciu, Chih-Yao Lin .............................................................................................. 727

Ways of Increasing the Efficiency of Refineries
Nickolai F. Kazichkin, Nikolai V. Lisitsyn, Vladimir I. Fedorov ...................... 728

Design of Divided Wall Reactive Distillation for Hydrolysis of Methyl Acetate
Hao-Yeh Lee, Hsiu-Ping Huang, Chih-Chun Hsu ........................................... 735

Investigation of Isobutene Dimerization Process in Reactive Distillation Using Rigorous Three-Phase Non-Equilibrium Stage Model
Amit Katariya, Marijana Chalakova, Hannsjorg Freund, Sanjay M. Mahajan, Kai Sundmacher ............................................................................. 736

Design of Ethanol Dehydration Process: Heterogeneous Azeotropic Distillation vs. Extractive Distillation
Lin Gunawan, I-Lung Chien ....................................................................... 737

A Non Linear Programming Formulation for Optimal Design of a Multitubular Packed Bed Reactor. - Simultaneous Solution: Case Study of o-Xylene Oxidation to Phthalic Anhydride
Carlos Andres Limas Vargas, Jorge Mario Gomez Ramirez ............................ 739

Analysis of Minimum Vapor Flowrate Requirements for the Fully Thermally Coupled Distillation System with Postfractionator
Lorena E. Ruiz-Martín, Angel Castrillo-Agüero, Nelly Ramírez-Corona, Arturo Jiménez-Gutiérrez ...................................................................................... 752

Composition Estimation of Reactive Distillation Systems and Its Implication to Feasibility
Joe W. Lee, James Chin .............................................................................. 762

The Study of Process Design for Production of the Clean Fuel – Dimethyl Ether (DME)
You-Syuan Chen, Jyun-Da Lin, Jhen-Ben Lee, An-Li Shieu, Jing-Jie Lan, Gow-Bin Wang .......................................................... 763

Web-Based Object-Oriented Modelling Environment for the Hierarchical Design and Simulation of Chemical Processes
Harvey Arellano-Garcia, Walter Martini, Stefan Kantche, Günter Wozny ......... 770

Use of Commercial Process Simulator to Mode Transition Control of the Tennessee Eastman Challenge Problem
Fei-Yu Lin, You-Syuan Chen, Gow-Bin Wang ............................................. 771

Experimental Studies and Optimal Design for a Small-Scale Autonomous Power System Based on Methanol Reforming and a PEM Fuel Cell
Martha Oszonoudou, Dimitris Ipatakis, Spyros S. Voutetakis, Simira A. Papadopoulos, Panos Seferlis ........................................................................ 777

Fadwa T. Eljake, Mario Richard Eden ....................................................... 785
A Molecular Signature Technique for Process and Product Design ................................................................. 787
  Nishanth Chemmangattuvalapil, Charles C. Solvason, Mario R. Eden

Systematic Integration of Process Attributes and Molecular Synthesis .......................................................... 788
  Charles C. Solvason, Nishanth Chemmangattuvalapil, Mario R. Eden

Byproduct Hydrogen Recycling Networks Design of Petrochemical Complex ................................................ 789
  Changhyun Jeong, Sangho Lee, Changhun Han

Development of Quantitative Structure-Property Relations for Ionic Liquids with Refrigerant Gases .......... 791
  SamanthA E. McLeese, Aaron M. Scarto, Kyle V. Camarda

A Novel Integrated Design of Wastewater and Heat Exchange Networks Based on Cost Estimation .......... 792
  Jiyoung Kim, Inkyung Kim, Youngeee Lee, Eunyong Kim, Il Moon

Global Sensitivity Analysis: Estimation of Sensitivity Indexes in Metabolic Network Dynamic Models .......... 793
  Jimena A. Di Maggio, Juan C. Diaz Ricci, Maria Soledad Diaz

Numerical Modeling of Horizontal Wafering of Silicon Melts on a Molten Substrate ................................ 794
  B. Erik Ydstie, Sukumar Balaji, Sudhir Ranjan

Optimal Design of Batch-Storage Network Under Joint Uncertainties ......................................................... 795
  Gyeongbeom Yi

MINLP Optimization of Cooling Towers ........................................................................................................... 806
  Medardo Serna-Gonzalez, Jose M. Ponce-Ortega, Arturo Jimenez-Gutierrez

Optimal Detailed Design for Integral Cooling Water Systems ........................................................................ 816
  Jose M. Ponce-Ortega, Medardo Serna-Gonzalez, Arturo Jimenez-Gutierrez

GTL (Gas to Liquids) Process Optimization Simulation Study ............................................................. 825
  Yong Heon Kim, Hounpang Yuen Lee, Ki-Won Jun, Hyunkyu Joo, Changhun Han, In Kyu Song

Retrofit of Heat Exchanger Networks Including Process Modifications ..................................................... 838
  Jose M. Ponce-Ortega, Arturo Jimenez-Gutierrez, Ignacio E. Grossmann

How Much Is the Pharmaceutical Industry Potentially Losing Due to Lack of Information Interoperability? .. 848
  Leaelaf M. Hailamuriam, Venkat VenkataSubramanian, Arun Giridhar

A Problem Solving Environment for Integrated Solvent and Process Design on the Grid ................................ 849
  Athanasios I. Papadopoulos, Patrick Linke

A Data Model Supporting Intelligent Search for Materials Research ............................................................ 851
  Stephen D. Stammatt, Balachandran B. Krishnamurthy, Amr Shehab, Tanu Malik, Leif Delgass, Steven R. Dunlop, James M. Caruthers

An Ontology Approach to Represent and Extract Process Synthesis Knowledge in High-Throughput Optimization .... 853
  Antonis Kokossis, Franjo Cecelja, Claudia Labrador-Darder, Patrick Linke

Cyberinfrastructure Roundtable .......................................................................................................................... 854
  Larry Megan

Comparison of Coal Based Hydrogen and Electricity Generation Process Under a Carbon Constrained Scenario ................................................................................................................................. 855
  Liang Zeng, Fanxing Li, Deepak Sridhar, Fei Wang, Hyung Bae Kim, L. -S. Fan

Modeling of Fouling in Crude Oil Pre-Heat Trains to Reduce Energy Losses and Carbon Emissions ............ 868
  Francesco Coletti, Sandro Macchietto

Modeling Multi-Stream Heat Exchangers with or without Phase Change for Simultaneous Optimization and Heat Integration ......................................................................................................................... 869
  Ravindra S. Kamath, Ignacio E. Grossmann, Lorenz T. Biegler

Mixed-Integer Bi-Objective Optimization Algorithm for Solving Energy Supply Chain Problems ............... 872
  Ali Ozturk, Metin Turkay

Minimum Capital Cost for a Heat Exchange Network Using the IDEAS Framework ........................................ 874
  Jorge Pena Lopez, Vasilios I. Manousiouthakis

Design of Hydrogen-on-Demand System from a Sodium Borohydride Hydrolysis Reaction ........................ 881
  Ai-Jen Hung, Cheng-Ching Yu, Yih-Hang Chen Sr., Shing-Fen Tsai, Yu-Ti Hsu, Jie-Ren Ku

Detailed Steady State Modeling of An Anode-Supported Solid Oxide Fuel Cell (SOFC) .............................. 886
  Sang Youp Chae, Dehongnu Bhattacharya, Raghunathan Rangaswamy

Modeling and Optimization of Polymer Electrolyte Fuel Cells .................................................................... 887
  Parag Jain, Lorenz T. Biegler, Myung S. Jhon

Rib-Channel Optimization for Flowfield Design of PEM Fuel Cells ............................................................... 888
  Shivakumar Kameswaran, Arun Pandy, Mallika Gummalla, Robert Darling

Bacterial Aerosol Neutralization by Shock Waves Using a Novel Impactor: Design, Computation and Experiments .............................................................................................................................. 889
  Patrick B. Sistlan, Lucas Madler, David Pham, Mengheng Li, Xinyu Zhang, Panagiotis D. Christofides

Prediction of the Focal Sites of Tissue Injury Caused by Reactive Gas Uptake In the Respiratory Tract ......... 890
  Banafsheh Keshavarzi, James Ultman, Ali Borhan

Eulerian Particle Tracking in Bifurcating Biofluids ............................................................................................ 891
  Clinton W. Wininger, Jeffrey Heys
Rheology of Adult Stem Cells and Modelling of Flow Induced Deformation

Alexandre J. S. Ribeiro, Ender A. Finol, Kris Noul Dahl

Dynamics and Bifurcation Analysis of the Heat-Shock Response In Eukaryotic Cells

Dimitrios I. Gerogiorgis

Quantitative Structure-Property Relationship Modeling of Skin Irritation

S. Golla, K. Verramsetty, B. J. Neely, S. F. Mudibally, R. L. Robinson Jr., K. A. M. Gasem

Multisite Phosphorylation: An Ultrasensitive Mechanism for Protein Degradation

S. Marjan Varedi K., Xiaoxia (Nina) Lin

Operational Planning of a Large-Scale Industrial Batch Plant Under Uncertainty

Peter M. Verdegae, Christodoulos A. Floudas

Verified Uncertainty Analysis In Modeling Nonlinear Bioreactor Dynamics

Joshua A. Enzner, Mark A. Stadtherr

Global Optimization of Multi-Parametric Milp Problems

S. N. Faisca, Konstantinos I. Kouramas, Efstratios N. Pistikopoulos

Computational Strategies for the Planning of Deepwater Oilfield Infrastructure Under Decision Dependent Uncertainty

Bora Tarhan, Ignacio E. Grossmann

Optimal Planning and Operation of Cryogenic Air Separation Columns Considering Uncertain Demands and Product Transitions

Yu Zhu, Carl D. Laird

Management of the Pharmaceutical R&D Using Stochastic Programming

Matthew Colvin, Christos T. Maravelias

Optimal Intermediate Storage Level Design for Continuous Production Systems Under Unit Failure Scenarios

Kristin M. Davies, Christopher L. E. Swartz

Dynamics and Control of Vapor Recompression Distillation

Sajit S. Jogwar, Michael Baldea, Prodromos Daoutidis

Model Predictive Control of Feed Flow Reversal In a Reverse Osmosis Desalination Process

Panagiotis D. Chrisafides, Alex Bartman, Charles McFall, Yoram Cohen

Networked Control and Scheduling of Distributed Energy Resources: Application to Biomass Gas-Fueled Fuel Cell Networks

Nael H. El-Farra, Yin Xu, Yulei Sun, Sathyendra Ghantasala

Incipient Fault Detection In Offshore Oil and Gas Production Platforms: Hybrid Electro-Mechanical Monitoring of Rotating Equipment

Sathish Natarajan, Rajagopalan Srinivasan, Ashwin Khambadkone

Successful Industrial Application of Robust Inferential Sensors for NOx Emissions Monitoring


Applying Advanced Process Control to Fccu in a Petroleum Refinery

Xiaoming Jin, Maying Yang

A History and View to the Future for Knowledge Management and Organizational Learning In the Process Industries

Yince Grassl

Sustainability through Knowledge Management

James B. Porter Jr.

Developing a Reporting System for Environmental Compliance

Janonna Alvarez

Understanding Root Causes of Abnormal Situations in Process Industries

Peggy A. Hewitt

The Importance of Human Factors in Control Systems and Knowledge Management

B. Wayne Bequette, William Bolker

Using Industry Consortiums for Knowledge Management and Technology Transfer

Ed Fiesinger

Quantifying Intrinsic Noise Effects In Biochemical Reaction Networks

Vassilos Soithopoulos, Yiannis N. Kaznessis

Linking a Mitotic Oscillator to the Extracellular Environment

Ryan Vargo, Kyriacos Zygowakiz

Designing Effective Trial Treatments against Cancerous Tumor Growth

Nemoy Rau, Ileana C. Carpen

Rapid Stochastic Simulation of Ultra-Coupled ChEmical Reactions

Ian J. Laurencz, Erdem Arslan

An Adaptive Scheme for Continuously Inferring Blood Glucose Using Noninvasive Inputs

Nidhi Bhandari, Derrick Rollins, Nisarg Vyas, Dave Andre

Stability and Structure of Amyloid-Forming Peptides from Computer Simulation

Jie Zheng
<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Safe Parking of Batch Processes</td>
<td>1019</td>
</tr>
<tr>
<td>Synergistic Improvement of Process Safety and Product Quality</td>
<td>1020</td>
</tr>
<tr>
<td>Development of a New Pattern Recognition Method and Its Application to Just-In-Time Modeling</td>
<td>1021</td>
</tr>
<tr>
<td>A New Algorithm for Spectrum Alignment by Maximizing Correlations among Signature Peaks</td>
<td>1023</td>
</tr>
<tr>
<td>Data Driven Neural Network Based Models of RO Desalination Plant Operation and RO Membrane Performance</td>
<td>1026</td>
</tr>
<tr>
<td>Rectification of Multiscale Data with Reliability Assessment to Guide External Data Procurement In Life Cycle Assessment</td>
<td>1027</td>
</tr>
<tr>
<td>Latent Variable Batch Predictive Control</td>
<td>1029</td>
</tr>
<tr>
<td>Fractal Scaling In Crude Oil Price Evolution Via Time Series Analysis of Historical Data</td>
<td>1032</td>
</tr>
<tr>
<td>A Framework for Generating An Optimal Set of Robust Product Design Alternatives</td>
<td>1034</td>
</tr>
<tr>
<td>The Virtual Product-Process Design Laboratory</td>
<td>1036</td>
</tr>
<tr>
<td>A Systematic Method for Integrating Product Attributes and Molecular Synthesis</td>
<td>1037</td>
</tr>
<tr>
<td>Effects of Solvent Selection In Optimal Separation Process Design and Controllability Properties Using a Nonlinear Sensitivity Analysis Approach</td>
<td>1038</td>
</tr>
<tr>
<td>Combined Property Clustering and GC+ Techniques for Process and Product Design</td>
<td>1040</td>
</tr>
<tr>
<td>Integrated Design of Self Heating Products and Processes</td>
<td>1041</td>
</tr>
<tr>
<td>Bioprocess Synthesis, Design and Analysis through a Group- Contribution Approach</td>
<td>1042</td>
</tr>
<tr>
<td>Simultaneous Optimization of Cyclic Hoist Scheduling and Water-Reuse Network Design for Environmentally Benign Manufacturing</td>
<td>1043</td>
</tr>
<tr>
<td>Global Optimization of Batch Direct-Recycle Networks</td>
<td>1044</td>
</tr>
<tr>
<td>Property-Based Optimization of Direct-Recycle Networks and Wastewater Treatment Processes</td>
<td>1047</td>
</tr>
<tr>
<td>Designing the Optimal Supply Chain for Biodiesel Production in Spain</td>
<td>1055</td>
</tr>
<tr>
<td>Optimal Model-Based Production Planning for Refinery Operations</td>
<td>1057</td>
</tr>
<tr>
<td>Planning Parent Seed Production</td>
<td>1059</td>
</tr>
<tr>
<td>Integrated Economic Optimization and Model Predictive Control of Bio-Fuel Production Plant</td>
<td>1060</td>
</tr>
<tr>
<td>Peninsular Malaysia Operation Gas Fields Flow Network Optimization Model</td>
<td>1061</td>
</tr>
<tr>
<td>Enabling Model Based Decision Making by Sharing Consistent Equation Oriented Dynamic Models Between Multiple Simulation and Optimization Environments</td>
<td>1062</td>
</tr>
<tr>
<td>Refinery LPG Transfer and Storage Scheduling, A Genetic Algorithm Approach</td>
<td>1091</td>
</tr>
<tr>
<td>Implementation of Predictive Functional Control on a High-Pressure Distillation Column</td>
<td>1093</td>
</tr>
</tbody>
</table>

Author Index

Ajay Lakshmanan, Ashok Bhakta, Gabriel Lopez-Calva, James Fielding, Ajay Modi, James Goom
Shahrul Azman Zainal Abidin, Wai Chong Low
Abdulrahman M. Alattas, Ignacio E. Grossmann, Ignasi Palou-Rivera
José M. Ponce-Ortega, Mahmoud El-Halwagi, Arturo Jiménez-Gutiérrez
Vikas Khanna, Bhavik R. Bakshi
José M. Ponce-Ortega, Mahmoud El-Halwagi, Arturo Jiménez-Gutiérrez
Elisabeth Capon, Gonzalo Guillén-Gosalbez, Laureano Jiménez-Esteller, Antonio Espuña
Abdulrahman M. Alattas, Ignacio E. Grossmann, Ignasi Palou-Rivera
Matt H. Bassett
Carl A. Schweiger, Bijan Sayyar-Rodzari
Shahriar Aftab Zainal Abidin, Wai Chong Low
Ajay Lakshmanan, Ashok Bhakta, Gabriel Lopez-Calva, James Fielding, Ajay Modi, James Goom
Roger Rocha, Marcas V. S. Poggi De Aragão
Bram Satriadarma, Harvey Arellano-Garcia, Guenter Wozny