Computing and Systems Technology Division

Core Programming Topic at the 2011 AIChE Annual Meeting

Minneapolis, Minnesota, USA
16-21 October 2011

Volume 1 of 2

ISBN: 978-1-61839-731-7

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.

Printed by Curran Associates, Inc. (2012)

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

An Overview of Cast Division Activities ..... N/A
Mahmoud El-Halwagi, B. Wayne Bequette

Computer Aided Solvent Selection and Design Framework 2
Igor Mitrofanov, Elisa Conte, Jens Abildskov, Gürkan Sin, Raifqul Gani

Classification of Chemical Production Scheduling Problems and Approaches, and a General Solution Framework 5
Sara Zenner, Christos Maravelias

Model Development and Control Strategies for Multicomponent Alloy Solidification Processes and Its Application to Solar Cell Manufacturing 7
German A. Oliveros, Ruochen Liu, B. Erik Ydstie, Sridhar Seetharaman

Modeling and Control of Aggregate Thin Film Surface Morphology Using Stochastic PDEs and a Patterned Deposition Rate Profile 9
Xinyu Zhang, Jianqiao Huang, Gangshi Hu, G. Orkoulas, Panagiotis D. Christofides

Himmelblau Award Presentation ..... N/A
David A. Kofke

Expertise In Chemical Process Modeling 11
Paul M. Mathias

Students Learn Fundamentals of Process Operations and Control Using Dynamic Simulator of An Integrated Gasification Combined Cycle (IGCC) Plant with CO2 Capture 12
Debangsu Bhattacharyya, Richard Turton, Stephen E. Zitney

Teaching Design Using the Cache Learning Resource Center 14
Warren D. Seider

Peer Evaluation In Chemical Engineering Design Through Wikis 15
Caryn L. Heldt

The Minnesota Years: An Advisor's Perspective ..... N/A
George Stephanopoulos

The Wisconsin Years: IMC and CAD ..... N/A
W. Harmon Ray

The Caltech Years: Resiliency and Controllability ..... N/A
Ignacio E. Grossmann

Nonlinear IMC to NMPC ..... N/A
Lorenz T. Biegler

The ETH Years: Hybrid Systems 20
Tariq Samad

Perspectives On Manfred Morari's Contributions ..... N/A
Thomas F. Edgar

Particle Based Multi-Scale Modeling of the Dynamic Response of Hexahydro-1,3,5-Trinitro-s-Triazine (RDX): Constant Energy Dissipative Particle Dynamics with Coarse-Grained Density Dependent Potentials 22
Joshua D. Moore, Sergei Izvekov, Martin Lisal, John K. Brennan

Temperature-Accelerated Molecular Dynamics Reveals That Insulin Can Undergo Large-Scale Conformational Reorganization On Binding to Its Receptor 24
Harish Vashisth, Cameron F. Abrams

Multiscale Modeling for Phospholipid Bilayer Simulations 25
Emily Curtis

A Coarse Grained Model of Inhibitors to Scavenger Receptor Uptake to LDL 26
Michael Tomasini, M. Silvina Tomassone

Multiscale Molecular Modeling of Fullerol-Dendrimer Complexes 27
Seung Ha Kim, Monica H. Lamm

Multiscale Modeling of Perfluoropolyether Lubricants with Functional Endgroups 28
Robert Smith, Pil Seung Chung, Lorenz T. Biegler, Myung S. Jhon

Nanoparticles At the Water-Decane Interface: Evidence of Emergent Behavior From Equilibrium Multi-Scale Simulations 30
Heng Fab, Alberto Striolo

Heuristic Design of Reaction/Separation Processes 31
William L. Luyben

Thermal Integration of Reboilers Positioned Close to the Pinch Point of a Process 32
D. Jantes-Jaramillo, G. T. Polley, T. Gundersen, M. Picon-Nuez

Exergetic Temperatures for Exergy Targeting 38
Danahe Marmolejo-Correa, Truls Gundersen

Economic Objective Function In Process Flow Sheet Optimization - Do We Know Everything about It? 40
Zorka Novak Pintaric, Mihael Kasaö, Zdravko Kravanja

Heat Exchanger Network Synthesis with Non-Isothermal Mixing Using a Stagewise Superstructure 43
Kefeng Huang, Eid Almutairi, Iftekar A. Karimi

Global Optimization of Mixed-Integer Quadratically-Constrained Quadratic Programs (QCQP) Through Piecewise-Linear and Edge-Concave Relaxations 45
Ruth Misener, Christodoulos A. Floudas

Multi-Variate, Multi-Term, and Multi-Constraint Relaxations for Global Optimization of Nonconvex NLPs and MINLPs with BARON 49
Nick Sahinidis, Aida Khajavirad

Black-Box Optimization Via Global Optimization of Surrogate Models 50
Satyajith Amaran, Nick Sahinidis

Convergence Rate of Convex Relaxations 52
Agustín Bompadre, Alexander Mitsos

Tight LP Relaxations for Optimization Problems with Nonlinear Parametric ODEs 53
Benoit Chachuat

Deterministic Global Optimization with Differential-Algebraic Equations Embedded 55
Joseph K. Scott, Paul I. Barton

A Debottlenecking Study for a Dehydration Column 57
Ahmed A. Youssef, Mohan Khadilkar

Fast NMPC Applied to Industrial High Purity Propylene Distillation 67
Gilvan A. G. Fischer, Lorenz T. Biegler

Multiobjective Optimization of a Spouted Bed Reactor 69
Ghanim M. Alwan, Stoyan Nedeltchev, Shreekanta Aradhya, Muthanna Al-Dahhan

A Multifaceted Experimental Design Investigation of Nodule Formation In Electroformed Parts In Compact Disc Plating Operations 101
Z. Otero Gephardt, John Heinzel

Molecular Models Using VBA to Optimize the Process of Petroleum Refining 102
Tatiane Gercina De Vilas, Cláudio Oller Do Nascimento, Jadson Paulino Alves Da Silva

Optimization and Thermodynamic Analysis of Mixed Refrigerant System In Ethylene Plants 109
Karthik Krishnadevarajan, Jian Zhang, Qiang Xu

Real Time Optimization of Industrial Gas Plants and Networks 111
Tong Li

The Role of Physical Property Databases in Ch. E. Education 112
Mordechai Shacham, Michael B. Cutlip, Michael Elly

Molecular Simulation Modules for Instruction In Thermodynamics, Transport, Kinetics, and Materials 121
David A. Kofke, Andrew J. Schultz

Teaching Molecular Dynamics and Monte Carlo Simulations: Lessons Learned From the Statistical Thermodynamics Workshops At the School of Advanced Studies In Applied Thermodynamics, Rio De Janeiro, Brazil 122
Edward J. Maginn, Frederico W. Tavares, Charlles R. A. Abreu, Jindal K Shah, Craig Tenney

Liquid/Vapor Equilibrium Via Equations of State for First Semester Sophomore Students 123
Daniel Forciniti

Integrating Computational Transport Phenomena Into the Undergraduate Engineering Curriculum 128
Charles A. Petty, Satish Muthu, Andre Benard

Engineering the Lymph Node Microenvironment with Controlled Release Polymer Particles for Enhanced Vaccination 129
Christopher M. Jewell, Sandra C. Bustamante Lopez, Darrell J. Irvine

Design and Characterization of Self-Assembling, Peptide-Based Biomaterials As Immunotherapeutics 131
Amanda Trent, Matthew J. Black, Colleen Olive, Matthew Tirrell

siRNA Based Gene Therapy In Alzheimer's Disease 132
Aparna Chaudhary, Sanjeev Garg

Identifying Novel Bacterial Proteases Involved In Enhanced Virulence During Chronic Infection 133
Logan Macdonald, Justin Nice, Sean O'Keefe, Bryan W. Berger

Interplay of Flow and Oncotically Active Solute Transport Across the Arterial Endothelium: Hydraulic Conductivity Masking and Relevance to Atherogenesis 134
Shripad D. Joshi, Kung-Ming Jan, David S. Rumschitzki

Molecularly Imprinted Polymeric Nanoparticles for Treating Viral Infections - A Synthetic Antibody Approach 136
Yen Wah Tong, Niranjani Sankarakumar

Breast Cancer CSC Display Novel In Vivo Imaging Features, Reminiscent of Development, During Early Tumor Progression 137
Natesh Parashurama, Neethan Lobo, Michael Clarke, Sanjiv Sam Gambhir

The Kinetics of Redox Reactions of Hexavalent Chromium and Trichloroethylene In Wastes Containing Both Contaminants 138
Jacob Mlusu, Ramesh Chawla

Kinetic Modeling of Gas-Phase Mercury Oxidation by Chlorine and Bromine In Combustion Effluents During Oxy-Combustion 139
Itsaso Auzmendi-Murua, Joseph W. Bozzelli

A Computational Model to Evaluate Solar Offset and Water Generation From Atmospheric Moisture Using Location-Specific Annual Climate Data 140
Dia Milani, Ali Abbas, Marwan Mokhtar, Matteo Chiesa

Toxicity of Flue Gas In Microalgae CO2 Mitigation Systems 141
Adriana Pacheco, Mario M. Alvarez, Javier Lara-Gil

Reducing Air Quality Impact From Plant Start-up Emissions by Integrating Air Quality Modeling and Plant Start-up Simulation 142
Jian Zhang, Qiang Xu, Thomas C. Ho
Modeling and Optimization of a Modified Claus Process As Part of An Integrated Gasification Combined Cycle (IGCC) Plant with CO2 Capture 143
Debangsu Bhattacharyya, Dustin D. Jones, Richard Turton, Stephen E. Zitney
Internal Model Control, Model Predictive Control, and Shell ..... N/A
Carlos E. Garcia, Daniel E. Rivera
MIMO Controllability and Decentralized and Plantwide Control ..... N/A
Sigurd Skogestad
State-Space and Robust Model Predictive Control ..... N/A
Mayuresh V. Kothare, Jay Lee
The Influence of MPC On Biomedical Control ..... N/A
Francis J. Doyle III
Control of Hybrid Systems ..... N/A
Francesco Borrelli
Rebuttal ..... N/A
Manfred Morari
Using Convex Nonlinear Relaxations In the Global Optimization of Nonconvex Generalized Disjunctive Programs 151
Juan P. Ruiz, Ignacio Grossmann
Parallel Solution of Large-Scale, Block-Structured, Nonlinear Programming Problems with Significant Coupling 153
Jia Kang, Johan Akesson, Carl D. Laird
COLIN: Optimization Infrastructure for Hybrid Algorithms 154
John D. Siirola, William E. Hart
Optimal Sensitivity Based On IPOPT 155
Rodrigo Lopez-Negrete, Hans Pirnay, Lorenz T. Biegler
Advances In Multi-Parametric Mixed Integer Linear Programming 156
Martina Wittmann-Hohlbein, Efstratios N. Pistikopoulos
From Time Representations In Scheduling to Hybrid Spatial Representations In 2-D Allocation Problems 157
Pedro M. Castro, Ignacio E. Grossmann
Passivity-Based Plantwide Control Design by Flowsheet Decomposition 159
Timothy P. McFarland, B. Erik Ydstie
A Graph Theoretic Approach for Model Reduction and Control of Complex Energy Integrated Process Networks 160
Sujit S. Jogwar, Seongmin Heo, Srinivas Rangarajan, Prodromos Daoutidis
Robust Quasi-Decentralized Control of Networked Process Systems Under Communication Scheduling 162
Yulei Sun, Nael H. El-Farra
Model Predictive Control of Nonlinear Singularly Perturbed Systems: Application to a Large-Scale Process Network 164
Xianzhong Chen, Mohsen Heidarinejad, Jinfeng Liu, Muñoz De La Peña, Panagiotis D. Christofides
Globally Optimal Control of Nonlinear Process Networks: Easier Than Globally Optimal Control of Nonlinear Processes 165
Zayna Alhusseini, Vasilios Manousiouthakis
A Safe-Parking Approach to Handle Partial Plant Shutdown 166
Siam Aumi, Miao Du, Prashant Mhaskar
Distributed Model Predictive Control for UK CO2 Capture, Transport and Storage Network 168
Alicia Arce, Niall Mac Dowell, Alejandro J. Del Real, Nilay Shah, Lourdes F. Vega
Reducing Specific Energy Consumption In Reverse Osmosis (RO) Water Desalination: An Analysis From First Principles 170
Mingheng Li
Study On Energy Consumption and Emission Generation for A Chemical Plant Under Different Start-up Strategies 171
Jie Fu, Chuanyu Zhao, Xiongtao Yang, Chaowei Liu, Qiang Xu, Kuyen Li, Dan F. Smith
Dynamic Optimal Well Placement In Oil Reservoirs 172
Mohammad Sadegh Tavallali, Kwong Meng Teo, Iftekar A. Karimi
Optimal Synthesis for the Feed-Water-Heater Network of a Pulverized Coal (PC) Power to Minimize Water Consumption 175
Juan M. Salazar, Urmila Diwekar
Dynamic Modeling for Ionic Liquid-Based Absorption Refrigeration Systems 176
D. Andrei Maces, Mark A. Stadtherr
Numerical Simulation of Flow Characteristic and Coking Analysis In An FCC Disengager 178
Wang Juan, Yu Mao, Jiangyun Wang
CFD Modeling of a Molten Slag Jet Free Surface Flow During Mineral Wool Fiberization 185
Dimitrios I. Gerogiorgis, Dimitrios Panias, Ioannis Paspaliaris
Scalable Stabilized FE Formulations for Simulating Turbulent Reacting Flows In Light Water Reactors 187
Roger P. Pawlowski, John N. Shadid, Tom M. Smith, Eric C. Cyr
Determination of An Accurate Reduction Method for Stochastic Chemical Kinetic Models with Applications In Synthetic Biological Design 188
Patrick Smadbeck, Yiannis N. Kaznessis
Dynamical Pathway Sensitivity Analysis for Biological Systems 189
Thanneer Malai Perumal, Rudiyanto Gunawan

Uncovering "Hidden" Variability and Dynamic Patterns: Strategies for Analyzing High-Dimensional Data Sets 192
Mary M. Staehle, Babatunde A. Ogunnaike, James Schwaber, Rajanikanth Vadigepalli

An Improved De Novo Peptide Sequencing Framework Using Decomposition and Integer Linear Optimization 193
Zukui Li, Richard C. Baliban, Christodoulos A. Floudas

A Fitness Index for Transplantation of Perfused DCD Rat Livers 195
Sinem Perk, Maria-Louisa Izamis, Herman Tolboom, Basak Uygun, Francois Berthiaume, Martin L. Yarmush, Korkut Uygun

Comparative Analysis of Transcriptome and Lipidome of RAW 264.7 and Primary Macrophages 197
Mano R. Maurya, Shakti Gupta, Eoin Fahy, Ashok Reddy Dinasarapu, Sean Li, Manish Sud, Shankar Subramaniam

Modeling the Synergistic Effects of Combination Therapy for Glioblastoma Multiforme 198
Matthew Browe, Francisco G. Vital-Lopez, Antonios Armaou

Nonsmooth Dynamic Optimization for Bioreactors with Flux Balance Models Embedded 200
Kai Hoeffner, Stuart Harwood, Paul I. Barton

Optimal Operation of a CO2 Capturing Plant for a Wide Range of Disturbances 202
Mehdi Panahi, Sigurd Skogestad

Minimizing the Energy and Demand Cost of Building Energy Systems Based On Economic MPC 203
Jingran Ma, S. Joe Qin, Tim Salsbury

Hierarchical Control of Networks Featuring Large Solvent Recycle 204
Sujit S. Jogwar, Ana I. Torres, Prodromos Daoutidis

Mathematical Modeling and Steady-State Analysis of a Proton-Conducting Solid Oxide Fuel Cell 205
Mona Bavarian, Masoud Soroush

Adaptive Subspace System Identification for CO2 Capture Processes 207
Ricardo Dunia, Gary Rochelle, S. Joe Qin

Systematic Methods for the Elimination of Redundant Life Cycle Assessment Metrics In the Multi-Objective Optimization of Industrial Processes 209
Nagore Sabio, Carlos Pozo, Gonzalo Guillén-Gosálbez, Laureano Jiménez, Ramkumar Karuppiah, Venkatesh Vasudevan, Nicolas Sawaya, John T. Farrell

Application of the Path Integration Formalism to Analysis of Activated Processes In Complex Molecular Systems 211
Dmitry I. Kopelevich

Coupling Ballistic Transport and Surface Reaction Models for Simulation of Atomic Layer Deposition Processes 212
Curtisha D. Travis, Raymond A. Adomaitis

Substrate-Induced Oscillatory Activity of An Enzyme Regulated by Multisite Phosphorylation 214
Ping Liu, Ioannis G. Kevrekidis, Stanislav Y. Shvartsman

Stochastic Modeling and Monte Carlo Simulation of Bacterial Disinfection: Generalized Approach 216
Andres Argoti, L. T. Fan, Ronaldo G. Maghirang, S. T. Chou

Molecular Thermodynamics Modeling of Water Equilibrium and Heat of Sorption In Human Stratum Corneum 217
Victor R. Vasquez, O. Hanbury, Charles Coronella

Predator-Prey Targeting In Porous Medium by Chemical Swarm Robots 218
Peter Grancic, Frantisek Stepanek

Global Optimization of Thermochemical-Based Coal, Biomass, and Natural Gas to Liquids Processes Via Lograthmic Partioning Schemes 219
Richard Baliban, Josephine A. Elia, Ruth Misener, Christodoulos A. Floudas

A New Algorithm for the Global Optimization of Property-Based Water Integration In Eco-Industrial Parks 221
Eusiel Rubio-Castro, José María Ponce-Ortega, M. M. El-Halwagi, Medardo Serna-González

Path Flow Indicators As Optimization Drivers In a Systematic Retrofit Methodology for Chemical Batch Processes 222
Stavros Papadokonstantakis, Andrea Anja Bumann, Konrad Hungerbühler

Computer Aided Flowsheet Design Using a Group Contribution Based Approach 224
Susilpa Bommareddy, Mario Richard Eden

A Modeling Approach to for Chemical Process Synthesis 225
Carlos A. Henao, Christos T. Maravelias

Biomass to Bio-Chemicals: Extractive-Reaction Processes for the Production of 5-Hydroxymethylfurfural 228
Ana I. Torres, Prodromos Daoutidis, Michael Tsapatsis

Molecular Simulation Studies On the Rheological Properties of Silica Nanoparticles Embedded In a Polyethylene Melt 229
Yangyang Shen, M. Silvina Tomassone

Long Glass Fiber Orientation In Extensional Flow 230
Kevin J. Meyer, Kevin C. Ortman, D. G. Baird

Hybrid Model and Application In the Study of Interfacial Properties of Nanocomposites 231
Jie Feng, Sadhan C. Jana

A More Realistic Model for the Study of Thermal Conductivity of Nanocomposites 232
Khoa N. D. Bui, Dimitrios V. Papavassiliou

New Insight Into the Reaction Mechanism of SiC Oxidation and Nitridation: A Density Functional Theory Study of β-SiC (001) Surface 233
Satyender Goel, Linda J. Broadbelt

Optimization and Control of Heteroepitaxial Surface Morphologies 234
Jacob McGill, Nasser Mohieddin Abukhdeir, Babatunde A. Ogunnaike, Dionisios G. Vlachos

Valuation of Chemical Processes Subject to Stochastic Price Uncertainty 236
Patrick Mousaw, Fernando Garcia, Fanghui Fan, Jeffrey Kantor

MPC and the Smart Grid: Optimal Operation and Transmission Expansion 237
Donald J. Chmielewski

Microalgae Bioreactor Control by Model Predictive Techniques 238
Javad Abdollahi, Stevan Dubljevic
Nanoscale Process Control Engineering 240
Raj Chakrabarti
Control of a Motor Intended Neural Prosthetic Finger Using a Network of Cortical Motor Neurons 241
Gautam Kumar, Nitish V. Thakor, Mayuresh V. Kothare
Characterizing the Pore Structure of Biochars: A New Approach Based On Multiscale Pore Structure Models and Reactivity Measurements 244
Hao Sun, Caroline A. Masiello, Kyriacos Zygourakis
Modeling and Simulation of Globular Protein Crystal Growth 246
Michael Nayhouse, Panagiotis D. Christofides, G. Orkoulas
Modeling Excitation Energy Transfer In Photosynthetic Systems: Application to Peridinin-Chlorophyll-Protein Complex In Dinoflagellates 247
William P. Bricker, Cynthia S. Lo
A Generalized Runge-Kutta Framework for Explicit Tau-Leaping Algorithms 248
Leonard A. Harris, James Faeder
Multiphysics Model of Diesel Injector Deposit Formation 249
Richard H. West, Amrit Jalan, William H. Green
Numerical Simulation of Fuel NOx and Thermal NOx Emissions from an Industrial Burner Using Biomass-Derived Producer Gas 251
Sujith Sukumaran, Song-Charng Kong
Kinetic Modeling of Solid-Gas Reactions At Reactor Scale: A General Approach 252
Loic Favergeon, Jacques Morandini, Michele Pijolat, Michel Soustelle
Multiscale Methodology for Prototyping of Porous Catalysts 260
Milos A. Marek
A Mixed-Integer Linear Programming Model for Optimizing the Scheduling and Assignment of Tank Farm Operations 261
Sebastian Terrazas-Moreno, Ignacio E. Grossmann, John Wassick
Integrated Operational Planning and Medium-Term Scheduling for Large-Scale Industrial Semicontinuous/Continuous Processes 263
Jie Li, Peter M. Verderame, Christodoulos A. Floudas
Integrated Scheduling and Dynamic Optimization of Batch Processes Using State Equipment Networks 266
Yisu Nie, Lorenz T. Biegler
A Mathematical Programming Based Approach to Biologic Manufacturing Scheduling, Planning, Design, and Analysis 268
Spencer D. Miller, Steve Harding, George Applequist, Donald Miller, Joseph Pekny
Scheduling As a Cornerstone of CPAS 269
Iiro Harjunkoski, Martin Hollender
Real-Time and Rigorous Dynamic Hoist Scheduling 270
Chuanyu Zhao, Jie Fu, Qiang Xu
Use of Principal Components with Parallel Coordinates In Solid Oxide Fuel Cells Fault Diagnosis 272
Ricardo Dunia, Thomas F. Edgar, Benjamin J. Spivey
Fault Detection and Diagnosis in the Statistics Pattern Analysis Framework 275
Hector Galicia, Jin Wang, Qinghua He
Online Fault Diagnosis During Startup of Distillation Process Using Artificial Immune System 277
Yiyang Dai, Jinsong Zhao
A New Gaussian Mixture Model Based Bayesian Inferential Monitoring Framework for Complex Chemical Processes 286
Jie Yu
Forecast Intervals In K-Steps-Ahead Prediction Modeling Under Continuous-Time Monitoring with Application to Blood Glucose Inference 287
Derrick K. Rollins Sr., Lucas Beverlin, Kaylee Kotz, Nisarg Vyas, Dave Andre
Automatic Grading of TFT-LCD Glass Substrates Based On Machine Vision 289
J. Jay Liu, Seongkyu Yoon
Design of a Centrifugal Separator for Olive Oil Extraction Via Multiphase Flow CFD Simulation 290
Dimitrios I. Gerogiorgis
Optimal Design of Ionic Liquid Entrainers for Extractive Distillation of Azeotrope Systems 292
Brock C. Roughton, John White, Raifqul Gani, Kyle V. Camarda
Design and Synthesis of Complex Distillation Networks with Hybrid Genetic Algorithm 294
Seon B. Kim, Andreas Linninger
A Systematic State-Space Superstructure Based Methodology for Batch Mass Exchange Network Design 295
Lijuan Li, Ruijie Zhou, Hongguang Dong
Turndown Control Structures for Distillation Columns 304
William L. Luyben, Patrick J. Robinson
Mathematical Modeling and Steady-State Analysis of a Hybrid Solid Oxide Fuel Cell 305
Mona Bavarian, Masoud Soroush
Optimized Gas Loop Design for Fischer-Tropsch Process 306
Debanjan Chakrabarti, Lin Wang, Arun Cherian, Arno De Klerk, Vinay Prasad
Decision Making for Unconventional Natural Gas Production: A Multivariate Analysis Approach 308
Srimoyee Bhattacharya, Michael Nikolaou

Controlled Variables Selection for a Gas-to-Liquids Process 310
Mehdi Panahi, Sigurd Skogestad
Modeling and Control of a Hybrid Renewable Energy System 312
Milana Trifkovic, Mehdi Sheikhzadeh, Khaled Nigim, Prodromos Daoutidis
Offset-Free Model Predictive Control of Vapor Compression Cycle 314
Matt Wallace, Prashant Mhaskar, John House, Tim Salsbury
Networked Predictive Control of Distributed Energy Systems with Adaptive Communication 316
Yulei Sun, Nael H. El-Farra
A Predictive Controller Design for Spatially Distributed Processes Using Adaptive Model Reduction 318
Sivakumar Pitchaiah, Antonios Armaou
Constrained Multi-Rate State Estimation Using NLP Sensitivity-Based Moving Horizon Estimation 320
Rodrigo Lopez-Negrete, Lorenz T. Biegler
Resource-Aware Model Predictive Control Using Adaptive Sampling 322
Ye Hu, Nael H. El-Farra
LMI-Based Multi-Model Predictive Control of An Industrial C3/C4 Splitter 324
Bruno D. O. Capron, Darci Odloak
Data-Based Modeling and Control of Nylon-6,6 Batch Polymerization 326
Siam Aumi, Brandon Corbett, Prashant Mhaskar, Tracy L. Clarke-Pringle
Lyapunov-Based Economic Model Predictive Control of Nonlinear Systems: Handling Asynchronous, Delayed Measurements and Distributed Implementation 328
Mohsen Heidarinejad, Jinfeng Liu, Panagiotis D. Christofides
Economic MPC with Infinite Horizon 330
Donald J. Chmielewski, Benjamin P. Omell
Optimal Multi-Scale Capacity Planning Under Time-Sensitive Electricity Prices for Continuous Power-Intensive Processes 331
Sumit Mitra, Ignacio Grossmann, Jose M. Pinto, Nikhil Arora
Integration of Scheduling and Control with Closed Loop Implementation 333
Jinjun Zhuge, Marianthi G. Ierapetritou
A New MILP/Discrete-Event Simulation Algorithm for Scheduling Automated Wet-Etching Stations 335
Pedro M. Castro, Adrián Aguirre, Luis Zeballos, Carlos Méndez
In-Depth Study and Comparison of S-Graph Framework and Precedence Based MILP Formulations for Batch Process Scheduling 338
Mate Hegyhati, Tibor Holczinger, Ferenc Friedler
Planning and Scheduling Under Uncertainties: Data Processing and Solution Strategy 341
Kailiang Tong, Yucheng Wu, Jiadong Xu, Yiping Feng, Gang Rong
Advanced Optimization In Petroleum Refinery Planning 343
Omar J. Guerra, Ariel Uribe Rodriguez, Sandra Milena Montagut, Laura Andrea Duarte, Javier David Angarita
Computational Performance of Big-M Formulations In Scheduling of Multipurpose Batch Plants 344
Esmael Reshid Seid, Thokozani Majozi
Active Fault Isolation of Nonlinear Process Systems 345
Miao Du, Prashant Mhaskar
Kalman-Based Fault-Tolerant Control (FTC) for a Pilot-Scale Cooling Loop 348
Kris Villez, Humberto Garcia, Craig Rieger, Venkat Venkatasubramanian
Monitoring and Reconfiguration of Sampled-Data Nonlinear Hybrid Process Systems with Actuator Faults 351
Ye Hu, Nael H. El-Farra
The Square-Root Unscented Kalman Filter for Leak Detection and Location In Natural Gas Pipelines 353
Weiting Tang, M. Nazmul Karim
Thermodynamic Models for Leak Detection and Inventory Verification of Natural Gas In Salt Cavern Storage 354
Russell A. Ogle, D. "trey" Morrison, Ryan J. Hart
Hyperspectral Imaging Based Sensing Archiectures for Particulate Solids Process Monitoring and Diagnosis 355
Silvia Serranti, Giuseppe Bonifazi
Soft Sensor Development of Batch Bioprocess Using Bayesian Inference Based Support Vector Regression 363
Jie Yu
Networked Control of Spatially Distributed Systems: Handling Communication Constraints and Delays 364
Zhiyuan Yao, Nael H. El-Farra
A Distributed Predictive Control Framework for Smart Grid Development 365
Wei Qi, Jinfeng Liu, Panagiotis D. Christofides
Distributed Model Predictive Control of Switched Nonlinear Systems 366
Mohsen Heidarinejad, Jinfeng Liu, Panagiotis D. Christofides
Coarse-Graining Dynamical Networks with Intrinsic Heterogeneities 367
Karthikeyan Rajendran, Andreas C. Tsoumanis, Andreas I. Reppas, Constantinos I. Siettos, Ioannis G. Kevrekidis
Proactive Emission Source Detection and Evaluation with Air Quality Monitoring Network 369
Tianxing Cai, Qiang Xu
Fate of Commensalistic Cultures In Identical Coupled Bioreactors 370
Satish J. Parulekar
Incorporating Sustainability Into the Design of Chemical Process: From Reaction Pathway Selection to Process Design 371
Kailiang Zheng, Helen Lou

Optimization of CO_2 Capture Process with Aqueous Amines – a Comparison of Two Simulation-Optimization Approaches 372
Aroonsri Nuchitprasittichai, Selen Cremaschi

A New Process for TiO2 Production 374
David R. Corbin, Keith W. Hutchenson, Stephen E. Lyke, Eugene M. McCarron III, Mark B. Shiflett, Charlie C. Torardi, Joseph J. Zaher

Low Temperature Hydrothermal Crystallization for a New TiO2 Process 375
Keith W. Hutchenson, Sheng Li, David R. Corbin, Charles C. Torardi, Eugene M. McCarron

Integration of Electroplating Process Design and Operation for Simultaneous Productivity Maximization, Energy Saving, and Freshwater Minimization 376
Chaowei Liu, Chuanyu Zhao, Qiang Xu

Design of Biofuel Additives Using Chemometric Modeling and Molecular Design Techniques 377
Subin Hada, Charles C. Solvason, Mario Richard Eden

Rule of Thumb for Simulating Biomass Pyrolysis In Packed Bed Reactor 379
Widya Wijayanti, Ken-Ichiro Tanoue, Takahiro Suetomi, Tatsuo Nishimura, Miki Taniguchi, Ken-Ichi Sasauchi

Uncertainty Set Induced Robust Linear and Mixed Inter Linear Optimization and Their Probabilistic Guarantees: New Results and Comparative Study 386
Zukui Li, Christodoulos A. Floudas

Nonconvex Generalized Benders Decomposition for Optimal Process Design and Synthesis Under Uncertainty 389
Xiang Li, Asgeir Tomasgard, Paul Barton

Development of Property Models with Uncertainty Estimate for Process Design Under Uncertainty 391
Amol Hukkerikar, Bent Sarup, Jens Abildskov, Gürkan Sin, Rafiqul Gani

A Chance-Constrained Framework for Optimization Under Uncertainty 393
Sebastian Werk, Tilman Barz, Günter Wozny, Harvey Arellano-Garcia

Scheduling of Crude Oil Operations Under Uncertainty: A Robust Optimization Framework Coupled with Global Optimization 395
Jie Li, Ruth Misener, Christodoulos A. Floudas

Optimal Planning of Flexible Process Networks Under Uncertainty with Stochastic Inventory 398
Fengqi You

A Hybrid Approach for Process Scheduling Under Uncertainty 400
Martina Wittmann-Hohlbein, Efstratios N. Pistikopoulos

Synthesis of Sustainable Property-based Water Networks 402
Luis Fernando Lira-Barragán, José María Ponce-Ortega, Medardo Serna-González, M. M. El-Halwagi

Comparing Continuous and Batch Process Design Under Uncertainty for Biodiesel Production 410
Pahola T. Benavides, Urmila Diwekar, Juan M. Salazar

Simultaneous Optimization of Flowsheet, Heat Recovery, and Water Network 411
Linlin Yang, Ignacio Grossmann

Incorporating Safety and Efficiency Considerations In Sustainability Assessment of Poly-Generation Systems 413
Preeti Gangadharan, Kailiang Zheng, Abhishek V. Jayswal, Anand Zanwar, Helen Lou

Technology Evaluation and Decision Making for Sustainability Enhancement of Industrial Systems Under Uncertainty 414
Zheng Liu, Yinlun Huang

Integration of Production Processes, Waste Management and Energy Utility Generation In Chemical Batch Plants 415
Stavros Papadokonstantakis, Claude Rerat, Konrad Hungerbühler

Economic Analysis of Municipal Wastewater Utilization for Thermoelectric Power Production 417
Iman Safari, Michael E. Walker, Javad Abbasian, Hamid Arastoopour, Ming-Kai Hsieh, Ranjani B. Theregowda, David A. Dzombak, David C. Miller

Modeling of Dynamic Hindered Diffusion of Drugs From Biodegradable PLGA Microspheres with Evolving Porous Structure 418
Ashlee N. Ford Versypt, Daniel W. Pack, Richard D. Braatz

Applications of Fractional Calculus to Anomalous Mass and Heat Transfer Phenomena In Complex Media 420
Ruben D. Vargas, Watson L. Vargas

Stress Distribution In Flow Through Porous Media 422
Naga Rajesh Tummala, Roman S. Voronov, Dimitrios V. Papavassiliou

Modeling Cellular Metabolism and U(VI) Immobilization In Shewanella Oneidensis MR-1 Biofilms 424
Bulbul Ahmed, Ryan S. Renslow, Haluk Beyenal

Retro-Convection Enhanced Drug Delivery: Computational Analysis and Pharmacodynamic Modeling 425
Daniel Lepek, Michael Cerro

An Area-Averaging Approach for Electrochemical Systems and It's Validity 434
Rajavardhan [raja] Reddy Nagolu, Vinten Diwakar, Pedro E. Arce

Mixing Improvement of Fluid Flow Using Lagrangian Coherent Structures 435
Mojtaba Izadi, Stevan Dubljevic

Suffocating On a Plastic Bag? Modeling Hypoxia In Porous Polymer-Cell Constructs 437
Roger L. York, Monica Neugebauer, Minglin Ma, Robert Langer, Daniel Anderson

Understanding the Evolution of by-Product Synergy Networks by Network Analysis 438
Shweta Singh, Bhavik R. Bakshi

Optimal Rerouting of Traffic Flows for Resilient Management of Recharging Station Networks 439
Kris Villez, Craig Rieger, Venkat Venkatasubramanian

Scheduling of Multiple Chemical Plant Start-Ups for Minimizing Regional Air Quality Impacts 441
Tianxing Cai, Qiang Xu

Assessing Risks Due to Loss of Natural Capital: The Case of Pollination Services 442
Vikas Khanna, Bhavik R. Bakshi
Supply Chain Planning In Oil & Gas Industry: Energy and Clean Technologies Under Uncertainty 444
Ivan Ordoñez Sr., Ariel Uribe, Andrés Joaquín Calderon
Designing Subsea Production Facilities for the Worst Case Using Semi-Infinite Programming 445
Matthew D. Stuber, Paul I. Barton
Rigorous Approach for Robust Design of Nonlinear Dynamic Systems 447
Yao Zhao, Mark A. Stadtherr
An Optimization-Based Framework for Process Planning Under Uncertainty with Risk Management 449
Cheng Seong Khor, Sara Giarola, Benoit Chachuat, Nilay Shah
Robust Optimization of the Capacitated Vehicle Routing Problem Under Demand Uncertainty 451
Chrysanthos E. Gounaris, Wolfram Wiesemann, Christodoulos A. Floudas
Managing Large-Scale Uncertainty In Process Flow Sheet Synthesis and Design 453
Mihael Kasa, Zdravko Kravanja, Zorka Novak Pintari
Improving Supply Chain Management In a Competitive Environment Under Uncertainty 456
M. Zamarripa, A. Espuna
Stochastic Programming and Uncertainty Management In Electricity System Operation 466
Bri-Mathias S. Hodge, Erik Ela, Michael Milligan
In-Silico Design of Experiments As a Tool for Nonlinear Sensitivity Analysis of Detailed Models 468
Alexandros Kiparissides, A. Mantalaris, Stratos Pistikopoulos, Christos Georgakis
In Silico Prediction of Cancer GI50 470
E. A. Whitebay, J. D. Ramsey, B. J. Neely, K. A. M. Gasem
A Mesoscopic Membrane Model for the Investigation of Mechanisms Underlying Caveolae-Mediated Endocytosis 471
Belinda S. Akpa, Richard D. Minshall, Lewis E Wedgewood, Ludwig C Nitsche
Modeling Heterogeneity In Populations of Self-Renewing Human Embryonic Stem Cells 472
Jincheng Wu, Emmanuel (Manolis) S. Tzanakakis
Systematic Engineering Approach to Development and Identification of Physiologically-Based Pharmacokinetic Models 473
Cierra Hall, Martina Heitzig, Gürkan Sin, Rafiqul Gani, Andreas Linninger
A Compartmentalized Sepsis Model Based On Neutrophil Kinetics As a Decision Supporting Tool of Therapeutic Intervention 475
Sang Ok Song, Justin S. Hogg, Robert S. Parker, Gilles Clermont
A Lattice-Based Computational Model of Microscopic Bone Resorption In Cortical Bone Multicellular Units 477
Junhwan Jeon, Pascal R. Buenzli, Peter Pivonka, David W. Smith, Peter T. Cummings
Optimal Control of Fed-Batch Fermentation Process Using Modified Iterative Dynamic Programming 478
Zheng Li, M. Nazmul Karim
Dynamical Analysis of Sucker-Rod String In Artificial Lift Systems for Control Applications 479
James C. Ng, Stevan Dubljevic
Plantwide Control of a Hybrid IGCC/Methanol Plant 480
William L. Luyben, Patrick J. Robinson
Optimization of Hydraulic Fracturing In Horizontal Wells for Unconventional Gas Production 481
Srimoyee Bhattacharya, Michael Nikolaou
Dynamic Modeling and Analysis of a Post-Combustion Carbon Dioxide Capture System 483
Zhixin Wang, Jianhong Lu, B. Wayne Bequette, Tiejun Zhang
Dynamic Modeling and Model-Based Control Strategy for Dimethyl-Ether (DME) Production Reactor 484
Yu Kyung Lim, En Sup Yoon, Jong Min Lee, Shin Je Lee, Sung Ho Kim
Studying Various Optimal Control Problems In Biodiesel Production In a Batch Reactor 486
Pahola T. Benavides, Urmila Diwekar
Model Predictive Control for Load-Following of An Integrated Gasification Combined Cycle (IGCC) Plant with CO2 Capture 487
Debangsu Bhattacharyya, Richard Turton, Stephen E. Zitney
Applying the Annular Flow Model to Complex Flow Systems 489
Ardson Do S. Vianna Jr., José Carlos G. Peres
Modeling of a Bubble-Train Flow and Interphase Mass Transfer In a Long Microchannel 497
Dmitry Eskin, Farshid Mostowfi, Shahnawaz Molla
Numerical Investigation of Mixing Inside the Dispersed Phase In Slug Flows In Microchannel 499
Yuehao Li, Rupesh Reddy, Krishnaswamy Nandakumar, Challa S. S. R. Kumar, Sanchita Biswas, Shuning Li
Pseudo-analytical Solution of the Power Law Model for For Non-newtonian Carrier Fluids in Free Convective Cells 505
Mario Oyanader, Patricio Trigo, Pedro E. Arce
Interaction Between An Elastic Filament and the Vesicle Membrane 506
Yuan-Nan Young, Christopher Jacobs
Implementing Chem-e-Car Competition Into the Curriculum: Ten Year Experience 507
Sundararajan. V. Madihally
Group Contribution Methods In Undergraduate Chemical Engineering Thermodynamics 508
Rebecca K. Toghiani
Browser-Based Simulations for the Illustration of Chemical Engineering Concepts 510
Anthony Butterfield
Shifts In Student Attitudes to a Technology-Based Active Learning Pedagogy 511
Milo D. Koretsky, Bill J. Brooks

Applying Reaction Engineering In a Virtual Chemical Company 512
Marcel A. Liauw, Steffen Heddrich, Volker L. Deringer
The Benefits of Using Computational Modeling In the Classroom to Complement Experiment 513
David Gallagher
Energy Modules for Hydrogen and Fuel Cells In the Chemical Engineering Curriculum 514
Jason Keith, Daniel Lopez Gaxiola, Daniel A. Crowl, Dave Caspary, Abhijit Mukherjee, Dennis Desheng Meng, Jeff Naber, Jeff Allen, John Lukowski, Barry Solomon, Jay Meldrum, Thomas F. Edgar
Optimal Operation and Design of Pooling and Other Bilinear Networks 515
Keith Zorn, Nick Sahinidis
Sizing Safety Stock for Supply Chain Risk Management: The Sole Source Disruption Risk 517
Russell A. Ogle, Mark J. Viz, Dennis M. McCann
A Holistic Framework for Drug Development and Capacity Planning In Novel Pharmaceutical Supply Chains 519
Arul Sundaramoorthy, James M. B. Evans, Paul I. Barton
Integrated Planning and Scheduling of Multisite Production and Distribution Facilities 521
Nikisha Shah, Marianthi Ierapetritou
Operability Considerations In Process Supply Chain Design for Forest Industry Transformations 524
Richard Mastragostino, Christopher L. E. Swartz
Planning and Long-Term Scheduling of Single-Stage Multi-Product Continuous Lines with a Complex Recycling Structure 527
Ricardo M. Lima, Ignacio E. Grossmann, Yu Jiao
Agent-Based Chemical Supply Chain Models Assessing Dynamic Disruptions 530
Mark Pepple, Amy Sun, Mark A. Ehlen, Brian S. Jones
A Comparative Study of Gray and Non-Gray Methods of Computing Gas Absorption Coefficients and Its Effect On the Numerical Predictions of Oxy-Fuel Combustion 540
Muhammad Sami, Pravin Nakod, Stefano Orsino, Gautham Krishnamoorthy
Energy Systems Integration Using Reduced Order Methods 554
Parag Jain, Lorenz T. Biegler, Myung S. Jhon
Distillation Column Conceptual Design In the Presence of Uncertain Parameter Using Bayesian Network 555
Farhang Jalali , Zahra Amini, Majid Nili
A Mathematical Programming Formulation for the Synthesis of Property-Based of Batch Water Network 562
José Antonio Vázquez-Castillo, José María Ponce-Ortega, Juan Gabriel Segovia-Hernández, M. M. El-Halwagi
Optimization of the Biofouling Control In Integrated Desalination/Power Plants 572
Fabricio Nápoles-Rivera, Abdullah Bin Mahfouz, Arturo Jiménez-Gutiérrez, M. M. El-Halwagi, José María Ponce-Ortega
Optimal Design of Distributed Treatment Systems for the Effluents Discharged to the Rivers 580
Oscar Burgara-Montero, José María Ponce-Ortega, Medardo Serna-González, M. M. El-Halwagi
Property-based Mass Integration Considering Efficient Property Operators 588
Ma Guadalupe Rojas-Torres, José María Ponce-Ortega, Medardo Serna-González, M. M. El-Halwagi
Development of Moving Bed Simulation Model for Carbon Capture From Fossil Energy Systems 589
Hosoo Kim, David C. Miller
Optimal Planning and Scheduling of a Biomass Conversion System Considering Economic and Environmental Aspects 590
José Ezequiel Santibañez-Aguilar, Janett Betzabe Gonzalez-Campos, José María Ponce-Ortega, Medardo Serna-González, M. M. El-Halwagi
Process Design: Principles and Methods - Process Design Project 598
Kate Harboe, Yu Jiang, Alessandra Pennati
Sustainable Integration of Industrial Gaseous Emissions 728
Pascual Eduardo Murillo-Alvarado, José María Ponce-Ortega, M. M. El-Halwagi, Juan Gabriel Segovia-Hernández
Sustainable Optimization of Steam Power Plants 740
César Giovani Gutiérrez-Arriaga, Medardo Serna-González, José María Ponce-Ortega
Simulation of a Typical and An Advanced Fischer Tropsch Reactor Technology 741
Marwan Abbas, Fadwa T. Eljack, Elfatih E. Elmalik, Aswani K. Mogalicherla, Nimir O. Elbashir
Production of Ethyl Alcohol From Excess Ethylene: A Systematic Approach for Conceptual Process Design 743
Thomas Bisgaard, Kim Braad Carlsen, Adam Samir Kadhim
Design for a Medium to Small-Scale Hydrogen Liquefaction Plant 827
Young Kim, Junseok Ko, Yong-Ju Hong, Kong Hoon Lee
Use of Surrogate Models In Water Network Synthesis 828
José Eduardo A. Graciano, Galo A. C. Le Roux
Simultaneous Environmental and Economic Optimization of Reverse Osmosis Plants Coupled with Solar Rankine Cycles 831
Gonzalo Guillén-Gosálbez, Raquel Salcedo-Díaz, Ekaterina Antipova, Dieter Boer, Laureano Jiménez
Combined Use of Simulation Packages, Multi-Objective Optimization and Statistical Tools for the Environmentally Conscious Design of Thermodynamic Cycles 832
Robert Brunet, Daniel Cortés, Dieter Boer, Gonzalo Guillén-Gosálbez, Laureano Jiménez
Effect of Salt Addition On Extractive Distillation Process 833
Russell Cruz, Nelly Ramírez, Luis Ríos, Arturo Jiménez
Dynamic Behavior of a Thermally Coupled Distillation Column Implemented On a Reactor-Separation-Recycle System 834
Daniel Mascote, Nelly Ramírez, Arturo Jiménez
Model Based Optimization of Bioethanol Production From Lignocellulosic Biomass 835
Federico Andersen, Susana Moreno, Maria Soledad Diaz

Eutrophication Control In Lakes and Reservoirs Through Integrated 3D Ecological and Hydrodynamic Models 837
Sabrina Belen Rodriguez Reartes, Vanina Estrada, Maria Soledad Diaz
Quantum-Level Descriptors In Computational Molecular Design 839
Qi Chen, Karen D. Camarda, Kenneth Bishop, Kyle V. Camarda
Characterization Based Molecular Design of Biofuel Additives for Feedstock Flexibility 840
Subin Hada, Charles C. Solvason, Mario Richard Eden
Group Contribution Based Process Synthesis and Design 842
Susilpa Bommareddy, Mario Richard Eden
Modeling and Optimization of a Multiple Tube Solar Receiver for High Temperature Solar-Thermal Processes 843
Janna Martinek, Carl Bingham, Alan W. Weimer
Simultaneous Linear and Nonlinear Approach to Solving Complex Mathematical Models In Chemical Engineering 845
Sreenivas Vemulapalli
Three-Dimensional Micro-Scale Model for Convective Drying 846
Abdolreza Kharaghani, Christoph Kirsch, Thomas Metzger, Evangelos Tsotsas
Multivariate Analysis and Reduced Order Modeling Based On Discrete Element Method (DEM) Simulations for a Powder Blender 855
Yijie Gao, Fani Boukouvala, Fernando J Muzzio, Marianthi G. Ierapetritou
A Quasi-Continuum Approach for the Computational Modeling of the Compaction of Bi-Layer Pharmaceutical Tablets – Prediction of Axial Tensile Strength 859
Athanas A. Koynov, Ilgaz Akseli, Alberto Cuitino
Mathematical Modeling of Intravascular Drug Delivery In Drug-Eluting Stents with Biodegradable Coating 860
Xiaoxiang Zhu, Richard Braatz
Derivation of Equations of State by Discrete Modelling of Entropy 862
Martin Pfleger, Thomas Wallek
Gap Gene Regulation In Drosophila: A Study In Multi-Objective Optimization of Spatiotemporal Models 863
James Hengenius, Michael Gribskov, Ann Rundell, David Umulis
Numerical Methods for a Case of Fractional Isoperimetric Problem 864
Annie X. W. Tangpong, Md. Mehedi Hasan
A New Global Optimization Algorithm and Its Application to Phase Stability Problems 865
Stanislaw K. Wasylkiewicz, Monika J. Wasylkiewicz
Optimal Control of Fed-Batch Fermentation Process Using Iterative Dynamic Programming 868
Zheng Li, M. Nazmul Karim
Tuning of Tabu Search Method for Optimal Scheduling Problems 869
William Bryant, Kyle V. Camarda
An Improved Kinetic Model of Mint Essential Oil Biosynthesis That Accounts for Transport and the Early Monoterpene Metabolic Steps 870
Daniel A. Carmona-Alvarez, B. M. Lange, Rigoberto Rios-Estepa, Rigoberto Rios-Estepa
A Fuzzy Sliding Mode Control Approach for Nonlinear Chemical Processes 871
Azar Shahraz
Mathematical Formulation of Carbon Capture and Storage Under the Presence of Uncertainty 872
Jun-Hyung Ryu, Jeehoon Han, In-Beum Lee
Optimal Design of Acid Gas Removal Unit In LNG Plant 873
Kiwook Song, Chul-Jin Lee, Jeongwoo Jeon, Chonghun Han
Design and Control of a Reactive Distillation Process for Naphtha Hydrodesulfurization 874
Ankit Sharma, Nitin Kaistha
Robust Averaging Level Control 876
Peter Rosander, Alf J. Isaksson, Johan Làfberg, Krister Forsman
Effect of Uncertainty In Time Delay On Multi-Step-Ahead Predication Performance of Some Black Box Models 883
Lemma D. Tufa, Marappagounder Ramasamy
Energy Network Dispatch Optimization Under Emergent Events of Local Energy Shortage 884
Tianxing Cai, Qiang Xu
Modeling and Control of the Solar Powered Membrane Distillation System 885
Jiann-Shiun Lin, Hsuan Chang, Gow-Bin Wang
The Square-Root Unscented Kalman Filter for Leak Detection and Identifying Location of Leaks In Natural Gas Pipelines 890
Weiting Tang, M. Nazmul Karim
Constrained Nonlinear State Estimation of An Acid Gas Removal Process As Part of An Integrated Gasification Combined Cycle (IGCC) Power Plant with CO2 Capture 891
Debangsu Bhattacharyya, Prokash Paul, Richard Turton, Stephen E. Zitney
Nonlinear Control of Dynamic Processes Using Models Based On Granular Runge-Kutta Methods 893
Tomas Co
Separating the Identifications of Nonlinear and Linear Parts In Block-Oriented Nonlinear Models Using Subspace Identification Approach 894
Jyh-Cheng Jeng
Model Predictive Control with Gradient of a Function of the Optimizing Targets 899
Luz Adriana Alvarez, Darci Odloak
Model-Based Sensor Placement for Component Condition Monitoring and Fault Diagnosis In Fossil Energy Systems 900
Jeevan Maddala, Babji Srinivasan, Debangsu Bhattacharyya, Richard Turton, Raghunathan Rengasamy

Mathematical Modeling of a Dye-Sensitized Solar Cell 901
Mona Bavarian, Siamak Nejati, Kenneth K. S. Lau, Masoud Soroush
The Use of a Time Variant IMC Controller for Robust Performance Improvement 903
Jonathan Whitlow, Latifat Adebayo
Energy Integration In Solid Oxide Fuel Cell Systems Under Different Steam Reformer Conditions: a Design and Control Approach 904
Dimitrios Georgis, Sujit S. Jogwar, Ali Almansoori, Prodromos Daoutidis
A New Method for the Global Optimization of Nonlinear Problems with Bilinear Terms 906
Joo Teles, Pedro M. Castro, Henrique A. S. Matos
CFD Simulation of Large-Scale Bioreactor with Side-Entry Agitator 908
Minhua Zhang, Yonghui Li, Zhiqiang Zhang, Jing Ma
Supply Chain Management Challenges In Continuous Pharmaceutical Manufacturing (CPM) 909
Dimitrios I. Gerogiorgis
Simulating the Impact of Distillation Operating Parameters On Energy Requirement for Methanol Separation From Biodiesel 911
Bipro Ranjan Dhar, Kawnish Kirtania
A Novel Technique for Prediction of Time Points for Scheduling of Multipurpose Batch Plants 912
Esmael Reshid Seid, Thokozani Majozi
SCONTO: A Supply Chain ONTOlogy That Extends and Formalizes the SCOR Model 920
Alicia C. Bàhm, Horacio P. Leone, Gabriela P. Henning
An Advanced Scheduling Technique for Multipurpose Batch Plants 923
E. Reshid, T. Majozi
Using Layer of Protection Analysis to Mitigate Supply Chain Risk 931
Russell A. Ogle, Dennis M. McCann, Mark J. Viz
Simultaneous Optimization of Hoist Scheduling and Production Line Arrangement 932
Chuanyu Zhao, Qiang Xu
Real-Time Data Estimation Method for LNG Terminal Using Conventional Process Simulator 934
Sangho Lee, Chul-Jin Lee, Sungwoo Cho, Jeongnam Kim, Chonghun Han, Youngsub Lim
Simulation Based Optimization of Ventilation Strategies for Subway Tunnel Fires 935
Kyungjun Park, Dongil Peter Shin, Ki Jun Lee
Application of Monitoring, Fault Detection and Diagnosis for Next-Generation Fire Detection 937
Dongil Peter Shin, Kyungjun Park, Ki Jun Lee
State Estimation with Delayed Measurements In Polymer Processes Using Unscented Transform Filters 938
Ruben Galdeano, Mariano Asteasuain, Mabel C. Sanchez
Automatic Generation of Optimal System Configurations and Maintenance Policies for Protective Systems 946
Chuei-Tin Chang, Edwin Wibisono
Multi-Threading Parallelism On Multi-Core Processor PC for Interval Analysis 948
Mark Stadtherr, Gang (Gary) Xu
Inversion of Perturbed Matrix: The Key Step towards Generic Parametric Programming 967
Rajab Khalilpour, Iftekar A. Karimi
Dynamics and Control of High Duty Counter-Current Heat Exchangers 968
Seongmin Heo, Sujit S. Jogwar, Prodromos Daoutidis
Control of the Detached Bridgman Crystal Growth Process 969
Andrew Yeckel, Prodromos Daoutidis, Jeffrey J. Derby
Output Feedback Control Design for Transport Reaction Processes with Partial Sensor Information 970
Sivakumar Pitchaiah, Antonios Armaou
Modeling Spatial Variations In Thin-Film Processing of Copper Oxide Films for Solar Energy Applications and Hydrogen Production 972
David Arana-Chavez, Raymond A. Adomaitis
Constrained Sensor Fault-Tolerant Control of Distributed Process Systems 980
Zhiyuan Yao, Nael H. El-Farra
Stability Condition and Discretization Scheme for the Population Balance 982
Juan Du, B. Erik Ydstie
Process Optimization of Bioethanol Production Via Hydrolysis of Switchgrass 983
Mariano Martín, Ignacio E. Grossmann
Optimization Framework for the Process Synthesis and Simultaneous Heat and Power Integration of a Thermochemical Coal, Biomass, and Natural Gas to Liquids Facility 987
Richard Baliban, Josephine A. Elia, Christodoulos A. Floudas
Process Synthesis of Biodiesel Production Plant Using Artificial Neural Networks As the Surrogate Models 989
Ismail Fahmi, Selen Cremaschi
An Integrated Biofuels Strategy: Catalytic Conversion of Lignocellulosic Biomass to Liquid Hydrocarbon Fuels 991
Sercan Murat Sen, Carlos A. Henao, Elif I. Gurbuz, David Martin Alonso, James A. Dumesic, Christos Maravelias
A Life Cycle-Based Analysis and Optimization Framework for Designing Sustainable, Multi-Product Biomass-to-Bioproducts Value Chains 993
Paritosh K. Sharma, Jose A. Romagnoli
Decomposition Strategy for the Global Optimization of Energy Polygeneration Systems 996
Yang Chen, Xiang Li, Thomas A. Adams II, Paul Barton
Tighter Integration Between Planning and Engineering Models At BP 998
Thomas L. Bowman, Don L. Glass, Kheng Lau, Ajay Lakshmanan

Scheduling for Performance-Decaying Cracking Furnace Operation with Consideration of Inherent Process Upset Reduction 999
Chuanyu Zhao, Qiang Xu
A New MINLP Model for Optimal Planning of Offshore Oil and Gas Field Infrastructure with Production Sharing Agreements 1001
Vijay Gupta, Ignacio E. Grossmann
Towards Continuous Operations In Pharmaceutical Manufacturing 1003
Arun Giridhar, Girish Joglekar, Venkat Venkatasubramanian, Gintaras V. Reklaitis
Optimal Measurement Selection for Controlled Variables for Kaibel Distillation Column 1004
Ramprasad Yelchuru, Sigurd Skogestad, Deeptanshu Dwivedi
A Comparative Study of Nonlinear CDU Models for Refinery Planning Optimization 1018
Abdulrahman M. Alattas, Ignacio E. Grossmann, Ignasi Palou-Rivera
Optimal Chlorine Booster Station Placement for Contamination Response In Water Distribution Systems Using Stochastic Programming 1021
Gabriel Hackebeil, Angelica V. Wong, Katherine A. Klise, William Hart, Carl D. Laird
Cause and Effect Dynamic Modeling of Real Processes Under Freely Existing Data Collection 1023
Derrick K. Rollins Sr., Stephanie Loveland, Peggy Lee, Yiying Khor
Adaptive Data-Based Model Predictive Control of Batch Systems 1025
Siam Aumi, Prashant Mhaskar
Data Mining of Historic Data for Process Identification 1027
Daniel Peretzki, Alf J. Isaksson, André C. Bittencourt, Krister Forsman
Calorimetric Estimation Employing Unscented Kalman Filtering for a Batch Emulsion Polymerization Reactor 1034
Franklin D. Rincon, Marcelo Esposito, Galo A. Carrillo Le Roux, Claudia Sayer, Pedro H. H. Araújo
Selection of Similarity Measure for Locally Weighted Partial Least Squares Regression 1038
Ryota Okajima, Sanghong Kim, Manabu Kano, Shinji Hasebe
Loss Method: A Static Estimator Applied for Product Composition Estimation From Distillation Column Temperature Profile 1040
Maryam Ghadrdan, Chriss Grimholt, Sigurd Skogestad, Ivar J. Halvorsen
Incremental Model Identification of Reaction and Mass Transfer Kinetics In a Liquid-Liquid Reaction System - An Experimental Study 1043
Nimet Kerimoglu, Marcel Picard, Adel Mhamdi, Lasse Grenier, Walter Leitner, Wolfgang Marquardt
A Computational Methodology for Learning Low-Complexity Surrogate Models of Processes From Experiments or Simulations 1045
Alison Cozad, Nick Sahinidis, David C. Miller
Manifold Learning Techniques and Model Reduction for Dissipative Dynamics 1046
Benjamin Sonday, Karthikeyan Rajendran, William Gear, Amit Singer, Ioannis G. Kevrekidis
Application of Singular Value Decomposition to Enhance Proper Generalized Decomposition In Mildly Non-Linear 2-D Partial Differential Equation Problems 1048
Stephen Edie, Antony N. Beris
ODE Model Parameter Identification Via Global Optimization Techniques 1050
Jeremy A. Conner, Vasilios Manousiouthakis
A Novel Computational Framework for Reactive Flow and Multiphysics Simulations 1051
James C. Sutherland, Tony Saad
Computing Interval Bounds On the Solutions of Nonlinear Index One DAEs 1052
Joseph K. Scott, Paul I. Barton
Discrete Particle Swarm Optimization for the Selection of Input Variables of Feed Forward Neural Networks 1053
Alex Kalos
Real-TimeWater and Energy Management In Power Plants and Implications In Electricity Markets 1054
Victor M. Zavala, Juan M. Salazar, Emil Constantinescu, Urmila Diwekar
Optimal Production Planning Under Time-Sensitive Electricity Prices for Continuous Power-Intensive Processes 1055
Sumit Mitra, Ignacio Grossmann, Jose M. Pinto, Nikhil Arora
Design of Networks for the Large-Scale Deployment of CO2 Capture, Transport and Storage Using Multi-Period Optimization Models: The Case for the Netherlands 1057
N. V. S. N. Murthy Konda, Nilay Shah, Nigel P. Brandon
Global Optimization for Refinery Operations Planning Using Complex Unit Models 1059
Miguel Bagajewicz, Mesude Ozturk, Duyquang Nguyen
Economic and Environmental Optimization of the Biomass-to-Biofuel Supply Chain In the Midwest 1060
W. Alex Marvin, Lanny D. Schmidt, Saif Benjaafar, Prodromos Daoutidis
Dimensionality Reduction Techniques Coupled with Multi-Objective Optimization Applied to the Design of Bioethanol Supply Chains In Argentina 1062
Gonzalo Guillén-Gosálbez
Modeling and Optimization of Next Generation Feedstock Development for Chemical Process Industry 1064
Selen Cremaschi
Computer Aided Flowsheet Synthesis and Design Under Uncertainty In Vegetable Oil Production 1065
Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani
Why Using Ontologies In Process Modelling 1068
Heinz A. Preisig
Model Generation: Massive Parallel Computations for the Next Generation of Biomedical Engineering Applications 1069
Andreas Linninger, Madhawa Hettiarachchi

Automatic Reaction Network Generation Using Chemo-Informatics 1070
Nick Vandewiele, Kevin M. Van Geem, Marie-Fran¡oise Reyniers, Guy B. Marin

Model Based Experimental Design and Parameter Estimation for An Industrial Hydrophobic Interaction Chromatography Step From a Quality by Design (QbD) Perspective 1072
Edward J. Close, Jeff Salm, Jennafer Lyons, Daniel Bracewell, Eva Sørensen

Linking Simulation Tools Using the Pharmahub Work-Flow Management Functionality 1073
José Miguel Laínez, Michael J. McLennan, Linas Mockus, Gintaras V. Reklaitis

Computer-Aided Design for a Demonstration-Scale Packed-Bed Tubular Reactor Producing Epichlorohydrin 1074
Woohyun Kim, Choamun Yun, Ki Taek Jung, Sunwon Park, Sae Heon Kim

Online Outlier Detection with a Bayesian Supervisory Approach for Recursive Soft Sensor Update 1082
Hector Galicia, Qinghua He, Jin Wang

MPC Performance Monitoring and Evaluation Principles 1084
Luo Ji, James B. Rawlings

Nonlinear State Estimation Using Parent and Nested Particles In Sequential Monte Carlo 1087
Sridhar Ungarala

A Novel Framework for Multi-Mode Process Modeling and Monitoring 1089
Zhibo Zhu, Zhihuan Song, A. Palazoglu

Data-Based Monitoring and Retuning of Low-Level PID Control Loops 1090
Akradej Leosirikul, David Chilin, Jinfeng Liu, Jim Davis, Panagiotis D. Christofides

Control Loop Performance Assessment Using Detrended Fluctuation Analysis 1091
Babji Srinivasan, Tim Spinner, Raghunathan Rengasamy

Fault Detection and Fault-Tolerant Control of Particulate Processes with Sampled and Delayed Measurements 1092
Trina Napasindayao, Nael H. El-Farra

Robust Hybrid Control of Nonlinear Process Systems Subject to Control and Communication Constraints 1094
Ye Hu, Nael H. El-Farra

Lyapunov-Based Model Predictive Control of Stochastic Nonlinear Processes 1096
Maaz Mahmood, Prashant Mhaskar

Exploiting Market Fluctuations and Price Volatility Through Feedback Control 1099
Christopher V. Rao, Donald J. Chmielewski

Multiple Model Predictive Control of Air Separation Unit As Part of IGCC Power Plant During Rapid Load Changes 1100
Priyadarshi Mahapatra, B. Wayne Bequette, Stephen E. Zitney

Modeling and Control of An Industrial Hydrocracker Using the Discrete and Continuous Lumping Methods and Model Predictive Control 1102
Yaman Arkun, Hasan Sildir, Ummuhan Canan, Berna Cakal, Dila Gokce, Emre Kuzu

Heat-Exchanger Bypass Control 1105
William L. Luyben

An Alternative Approach to Online Model Identification and PID Controller Tuning 1106
Nataliya Baran, Günter Wozny, Harvey Arellano-Garcia

A Multi-Objective Mixed-Integer Dynamic Optimization Approach to Oil Spill Response Planning 1108
Fengqi You, Zhixia Zhong

Simultaneous Design and Control of Pressure Swing Adsorption Processes 1110
Harish Khajuria, Stratos Pistikopoulos

An Economic Nonlinear Model Predictive Control Formulation for Gas Pipeline Optimization 1112
Ajit Gopalakrishnan, Lorenz T. Biegler

Age Dependent Dynamic Operational Risk Assessment 1114
Shubharthi Barua, Xiaodan Gao, M. Sam Mannan

Simulation Based Optimization of Expensive Flowsheet Models for Continuous Pharmaceutical Manufacturing 1117
Fani Boukouvala, Marianthi G. Ierapetritou

Global Optimization of Nonsmooth Dynamic Systems 1120
Kamil A. Khan, Mehmet Yunt, Paul I. Barton

Global Optimization of Detailed Non-Linear Kinetic Models of Metabolic Networks Through Recasting Into Canonical Power-Law Representation 1122
Carlos Pozo, Gonzalo Guillén-Gosálbez, Laureano Jiménez, Albert Sorribas

Optimization of IGCC with CFD Based ROM 1124
Yi-Dong Lang, Stephen E. Zitney, Lorenz T. Biegler

Optimal Design of Oxy-Fuel Combustion for Carbon Capture and Sequestration 1125
Hussam Zebian, Nicholas D Mancini, Alexander Mitsos

Modeling and Optimization of Cathode Layer Microstructures In Polymer Electrolyte Fuel Cells 1126
Sesha Hari Vemuri, Parag Jain, Myung S. Jhon, Lorenz T. Biegler

Exergy-Based Optimization for Mixed Refrigerant Systems 1128
Jian Zhang, Meiqian Wang, Qiang Xu, Kuyen Li

Design of the Smart Community Through the Use of EV In a University 1129
Yuu Notoji, Kazuya Shimohara, Tsuguhiko Nakagawa

Design of a Self-Supporting Natural Gas Liquefaction Process for Accessing Stranded off-Shore Resources 1133
Achim Wechsung, Audun Aspelund, Truls Gundersen, Paul I. Barton

A Multi-Scale Model-Based Approach to the Synthesis and High-Throughput Analysis of Biorefineries 1134
Marinella Tsakalova, Aidong Yang, Antonis Kokossis

Stability Conditions for Adaptive Inventory Control Systems 1135
Juan Du, B. Erik Ydstie

Data-Driven Network Reconstruction of Biological Systems: Comparison of Statistical and Optimization-Based Methods 1136
Behrang Asadi, Mano R. Maurya, Daniel M. Tartakovsky, Shankar Subramaniam
A System Identification and Control Engineering Approach for Designing An Optimized Treatment Plan for Fibromyalgia 1138
Sunil Deshpande, Naresh N. Nandola, Daniel E. Rivera, Jarred W. Younger
Experimental Design of Systems Involving Multiple Fluorescent Reporters 1141
Loveleena Bansal, Eric Yang, Randall Nelson, Arul Jayaraman, Juergen Hahn
Subject-Specific Multiple Input Block-Oriented Glucose Modeling of Several Type 1 Diabetic Subjects 1143
Derrick K. Rollins Sr., Kaylee Kotz, A. Cinar, Elizabeth Littlejohn, Lauretta Quinn
Equilibrium Conditions In Tumors Undergoing Virotherapy 1145
Ricardo Dunia, Thomas F. Edgar
Model Based Control for Metabolic Shift Regulation In Mammalian Cells 1147
Damian Baeza, J. Cristian Salgado, Ziomara P. Gerdtzen
The Cascade Algorithm: a New Approach for Distributed Markov-Based Optimization 1152
Antonis Kokossis, Patrick Linke, Siyu Yang
High Performance Prediction of Molten Steel Temperature Through Gray-Box Model 1153
Toshinori Okura, Manabu Kano, Shinji Hasebe, Hiroshi Kitada, Noboru Murata
Performance Monitoring of Industrial Plant Alarm Systems Using Event Correlation Analysis 1155
Tsutomu Takai, Masaru Noda
Event Correlation Analysis of Plant Operation Data with Large Variance In Time Lag for Alarm System Rationalization 1157
Masaru Noda, Kohjiro Kurata, Yasunori Kikuchi, Masahiko Hirao
Operational Level Integration System Based On An Ontological Framework by Means of Master/Control Recipe Semantic 1159
Edrisi Muñoz, Elisabet Capon, Antonio Espuña, Luis Puigjaner
Descriptor-Based Models From High Throughput Research Workflows for Architectural Coatings 1161
Jonathan D. Moore, Guido Smits, Alan Chaput Jr.
Design of Experiments Based On Computational Singular Perturbation 1162
Siddhartha Kumar, Vinay Prasad
Exploring Protein-Excipient Interactions for Optimal Design of Protein Stabilizers 1163
Brock C. Roughton, Anthony I. Pokphanh, E. M. Topp, K. V. Camarda
Comprehensive Computer-Aided Molecular Design Framework for Pure Component Design 1165
Apurva Samudra, Nick Sahinidis
Systematic Molecular Design of Biofuel Additives Using Hybrid Characterization and Group Contribution Based Techniques 1167
Subin Hada, Charles C. Solvason, Mario Richard Eden
Multiscale Approach to Colloidal Systems (Emulsions) Design 1169
Andrea Nieto, Diego Pradilla, Natalia Murcia, Oscar Alvarez
Teaching Chemical Product Design 1171
Ed Cussler, Geoff D. Moggridge
Automated Real-Time Diagnostics of Model Predictive Control Actions 1173
Aditya Kumar, Michael Nikolaou
Economic Cost Function Design and Model Predictive Control of a Chemical Process Network 1175
Xianzhong Chen, Mohsen Heidarinejad, Jinfeng Liu, Panagiotis D. Christofides
Risk Analysis In the Process Industries: A Perspective 1176
Ankur Pariyani, Warren D. Seider, Ulku Oktem, Masoud Soroush
A Systematic Methodology for the Assessment and Troubleshooting of Control Strategies and Operational Problems In Distillation Systems 1177
Miguel Mauricio-Iglesias, Kristoffer Johansen, Sten Bay Jørgensen, Gürkan Sin
Automatic Generation of Emergency Response Procedures for Batch Processes 1179
Chuei-Tin Chang, Ming-Li Yeh
Plantwide Control for Economically Optimal Operation of An Ethyl Benzene Process 1180
Ashok S. Pathak, Nitin Kaistha
Author Index