

Computing and Systems Technology Division 2016

Core Programming Area at the 2016 AIChE Annual Meeting

San Francisco, California, USA
13 - 18 November 2016

ISBN: 978-1-5108-3432-3

Printed from e-media with permission by:

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



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

Copyright© (2016) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2017)

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

AIChE
120 Wall Street, FL 23
New York, NY 10005-4020

Phone: (800) 242-4363
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: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

(8w) Smart City, Smart Energy, Smart Decision Making	1
<i>Xiaonan Wang</i>	
(8x) Solution Approaches for Large Scale Multistage Stochastic Programs with Endogenous and Exogenous Uncertainty	3
<i>Brianna Christian</i>	
(8a) Multi-Scale Process Systems Engineering	4
<i>Bruno A. Calfa</i>	
(8b) Petroleum Coke Morphology Mapping: A Mechanistic Approach Using Machine Learning	7
<i>Pedro Amorim</i>	
(8c) Simulation and Optimization of Chemical Processes for CO₂ Sequestration and New Clean Energy: Cyclic Adsorption Process, Membrane, and Direct Methanol Fuel Cell	8
<i>Daeho Ko</i>	
(8f) Simulation of the Oil-Treatment Process in the Oil Sands Plant	9
<i>Choon H. Kang, Jin S. Heo, Moon Jeong</i>	
(8g) Effects of the Mixed Refrigerant Composition on the Performance of the Rankine Cycle Driven By LNG Cold Energy	10
<i>Choon H. Kang, Moon Jeong, Jin S. Heo</i>	
(8i) Process System Engineering for Advanced Modular Continuous Pharmaceutical Manufacturing Platform	11
<i>Ravendra Singh</i>	
(8j) Optimization-Based Quantification of Performance Limits for Process Networks	17
<i>Flavio da Cruz</i>	
(8k) Metabolic Modeling for Improved Bioprocess Efficiency	18
<i>Peter St. John</i>	
(8l) Dynamics of Discrete Systems: At the Interface of Engineering and Medicine	19
<i>Anwasha Chaudhury</i>	
(8m) Application of Modeling and Optimization Methods in Biomedicine and Biorefineries	24
<i>Kirti Maheshkumar Yenkie</i>	
(8n) Advanced Adaptive Control Approaches for Complex Batch or Semi-Batch Operations	27
<i>Vinay Bavdekar</i>	
(8o) New Modeling and Decision-Making Paradigms in Systems Engineering	30
<i>Alexander W. Dowling</i>	
(8p) Management of Energy Supply Chains Under Uncertainty	33
<i>Omar J. Guerra, G. V. Reklaitis</i>	
(8q) Energy Systems Analysis to Enable a Sustainable Economy	36
<i>Emre Gençer</i>	
(8s) Deterministic and Robust Model-Based Strategies for the Online Multi-Level Optimization of Batch Operations	37
<i>Francesco Rossi, Gintaras V. Reklaitis, Flavio Manenti, Guido Buzzi-Ferraris</i>	
(8y) Modeling and Control of Hybrid and Nonsmooth Process Systems	38
<i>Peter G. Stechlin</i>	
(8r) Energy Security and Environmental Protection: Bridging the Gap Between Theory and Application	41
<i>Mahdi Sharifzadeh</i>	
(8aa) Automatic Exploration of Potential Energy Surfaces: Towards Reaction Mechanisms, Rate Constants, and Product Branching Ratios From First Principles	44
<i>Adeel Jamal</i>	
(22a) Economic Model Predictive Control for Integrating Scheduling and Dispatch of Microgrid Power Systems	47
<i>Michael Zachar, Prodromos Daoutidis</i>	
(22b) Moving Horizon Closed-Loop Scheduling of Processes Operating Under Dynamic Constraints	48
<i>Richard Pattison, Cara Touretzky, Iiro Harjunkoski, Michael Baldea</i>	
(22c) The Control of Self-Interested Agents: Learning from Nature's Wisdom of Crowds	49
<i>Yu Luo, Garud Iyengar, Venkat Venkatasubramanian</i>	
(22d) Subspace Based Quality Control of Variable Duration Batch Processes	50
<i>Brandon Corbett, Prashant Mhaskar</i>	
(22e) Optimization Models for Shale Gas Development Planning: A Real-World Marcellus Shale Case Study	53
<i>Markus G. Drouven, Ignacio E. Grossmann</i>	
(22f) A Theoretical and Computational Study of Continuous-Time Process Scheduling Models in the Context of Adjustable Robust Optimization	55
<i>Nikolaos Lappas, Chrysanthos E. Gounaris</i>	
(22g) Decision Making Under Uncertainty in Integrated Planning of Generation and Transmission Capacities in Interconnected Power Systems	58
<i>Omar J. Guerra, Diego Tejada, Gintaras V. Reklaitis</i>	
(22h) An Efficient Method for Deriving Normalization Constants for Eigenfunctions of Sturm-Liouville Problems and Its Application to the Graetz Problem for Diffusive and Convection Heat/Mass Transfer	59
<i>Joel Paulson, T. Alan Hatton, Richard Braatz</i>	

(27a) Systematic Framework for Carbon Dioxide Capture and Utilization Processes to Reduce the Global Carbon Dioxide Emissions	60
<i>Rebecca Frauzem, Cristina Calvera Plaza, Rafiqul Gani</i>	
(27b) Design of Energy Saving CO₂ Separation Process Using Circulating Fluidized Bed	62
<i>Yasuki Kansha, Masanori Ishizuka, Hiroyuki Mizuno, Atsushi Tsutsumi</i>	
(27c) Systems Design and Economic Analysis of Direct Air Capture of CO₂ through Temperature Vacuum Swing Adsorption on Metal Organic Frameworks	63
<i>Anshuman Sinha, Lalit A. Darunte, Christopher W. Jones, Yoshiaki Kawajiri, Matthew Realf</i>	
(27d) New Performance Indicators for Adsorbents Used in CO₂ Capture Swing Adsorption Processes	64
<i>Seongbin Ga, Hong Jang, Jay H. Lee</i>	
(27e) Optimal Retrofit of a Post Combustion CO₂ Capture Process Using Reduced Superstructure and Rate-Based Models	65
<i>Ung Lee, Alexander Mitsos, Chonghun Han, Changsoo Kim</i>	
(27f) Dynamic Modeling with Uncertainty Quantification of Solid Sorbent Based CO₂ Capture Processes	66
<i>Anca Ostace, Debangsu Bhattacharyya, Keenan Kocan, David Mebane</i>	
(27g) CO₂ Capture and Conversion to Chemicals Via Syngas: Rigorous Modeling, Intensification, and Superstructure-Based Process Synthesis	67
<i>Priyadarshini Balasubramanian, Ishan Bajaj, M. M. Faruque Hasan</i>	
(28a) Efficient Estimation of Maximum Theoretical Productivity from Batch Cultures Via Dynamic Optimization of Flux Balance Models	68
<i>Peter St. John, Michael F. Crowley, Yannick J. Bomble</i>	
(28b) Computing Sensitivities for Nonsmooth Differential-Algebraic Equations	69
<i>Peter G. Stechlinski, Paul I. Barton</i>	
(28c) Evolutionary Optimization Environment for Power Plant Control with Dynsim® Interface	70
<i>Ghassan Al-Sinbol, Mario Perhinschi, Debangsu Bhattacharyya</i>	
(28d) Shale Gas Supply Chain Network Design and Operation Incorporating Rigorous Well Simulations	71
<i>Jorge Chebeir, Hope Asala, Aryan Geraili, Arash Dahi Taleghani, Jose Romagnoli</i>	
(28e) Dynamic Optimisation of Beer Fermentation: Sensitivity Analysis of Attainable Process Performance Vs. Product Flavour Constraint Levels	79
<i>Alistair D. Rodman, Dimitrios I. Gerogiorgis</i>	
(28f) Dynamic Optimization of Constrained SEMI-Batch Processes Using Pontryagin'S Minimum Principle – An Effective Quasi-Newton Based Approach	80
<i>Erdal Aydin, Kai Sundmacher</i>	
(28g) A Parallel Interior Point Solver with Cyclic Reduction for Solving Large-Scale Dynamic Optimization Problems	81
<i>Bethany Nicholson, Shivakumar Kameswaran, Thomas A. Badgwell, Lorenz T. Biegler</i>	
(28h) Computation of Sensitivities of Dynamic Systems with Lexicographic Linear Programs Embedded	82
<i>Jose A. Gomez, Paul I. Barton</i>	
(42a) Distributed Lyapunov-Based Model Predictive Control with Safety-Based Constraints	83
<i>Fahad Albalawi, Helen Durand, Panagiotis D. Christofides</i>	
(42b) Supervisory Event-Based Control of Networked Process Systems with Limited State Measurements	84
<i>Da Xue, Nael H. El-Farra</i>	
(42c) Distributed Extremum Seeking Control Over Unknown Network	87
<i>Judith Ebegebulem, Martin Guay</i>	
(42d) Power Management in Microgrids with Controllable Loads and Energy Exchange Commitments	88
<i>Michael Zachar, Prodromos Daoutidis</i>	
(42e) Forming Distributed Estimator Networks From Decentralized Estimators	89
<i>Xunyuan Yin, Jinfeng Liu</i>	
(42f) Coarse Modeling of Circadian Rhythms in Heterogeneous Neural Networks	90
<i>Tom S. Bertalan, Ioannis G. Kevrekidis</i>	
(42g) Dynamic Real-Time Optimization of Distributed MPC Systems	91
<i>Mohammad Z. Jamaludin, Christopher L. E. Swartz</i>	
(74a) Overview of CAST Activities and Programming	94
<i>Nick Sahinidis, Karl Schnelle</i>	
(74b) Towards a Computational Platform for General Flowsheet Synthesis	95
<i>Qi Chen, Ignacio E. Grossmann</i>	
(74c) Distributed Modifier-Adaptation Schemes for the Real-Time Optimization of Interconnected Systems in the Presence of Structural Plant-Model Mismatch	98
<i>René Schneider, Predrag Milosavljevic, Dominique Bonvin</i>	
(74d) GOSSIP: Decomposition Software for the Global Optimization of Nonconvex Two-Stage Stochastic Mixed-Integer Nonlinear Programs	101
<i>Rohit Kannan, Paul I. Barton</i>	
(74e) Dimensionality Reduction of Dynamic Networks	102
<i>Alexander Holiday, Assimakis Kattis, Balázs Ráth, I.G. Kevrekidis</i>	
(74f) Robust Dynamic Principal Component Analysis Method for Modelling Process Data	103
<i>Alisha Deshpande, S. Joe Qin, Lisa A. Brenskelle</i>	
(134a) Nonsmooth Models and Methods in Chemical Engineering	104
<i>Kamil A. Khan, Harry A. J. Watson, Paul I. Barton</i>	
(134b) Perspectives on Predictive Control with Dual Control Feature for Stochastic Systems	105
<i>Ali Mesbah</i>	

(134c) Mathematical Modeling at the Food-Energy-Water Nexus	106
<i>Kyriacos Zygourakis</i>	
(134d) Towards Systems-Scale Dynamic Metabolic Modeling	107
<i>Mark P. Styczynski, Robert Dromms</i>	
(134e) Modeling Convergence of Circadian Clocks and Metabolism	108
<i>Seul-A Bae, Ioannis P. Androulakis</i>	
(134f) Pore-Pore and Pore-Edge Interactions in Graphene Sheets and Nanoribbons	111
<i>Lin Du, Dimitrios Maroudas</i>	
(142a) Mathematics for Data-Driven Modeling - The Science of Crystal Balls	112
<i>Ioannis G. Kevrekidis</i>	
(142b) Decoding Common Features of Protein-Nanoparticle Interactions	113
<i>Qing Shao, Carol K. Hall</i>	
(142c) Design of Optimal Experimental Probes for Protein Dynamics Using Machine Learning and Variational Approach to Modeling Conformational Kinetics	114
<i>Balaji Selvam, Shriyaa Mittal, Chuankai Zhao, Divakar Shukla</i>	
(142d) Guiding Experiments Towards New Functional Materials with Informatics	115
<i>Prasanna V. Balachandran, Dezhen Xue, Turab Lookman</i>	
(142e) Pushing the Frontiers of Atomistic Modeling Towards Predictive Design of Materials	116
<i>Subramanian Sankaranarayanan, Badri Narayanan, Mathew Cherukara</i>	
(142f) Design of Ternary Transparent Conducting Oxides	117
<i>Christopher Sutton, Matthias Scheffler, Luca M. Ghiringhelli</i>	
(142g) Development of Empirical Charge Transfer Interatomic Potential for Tantalum Oxide Nanostructures from First Principle Calculations	118
<i>Kiran Sasikumar, Badri Narayanan, Subramanian K.R.S. Sankaranarayanan</i>	
(142h) Machine Learning for Advancing Discovery of Novel Thermoelectric Materials. The Thermoel	119
<i>Al'ona Furmanchuk, Ankit Agrawal, James Saal, Jeff Doak, Gregory Olson, Alok Choudhary</i>	
(142i) Identifying Descriptors for Dielectric Breakdown Strength Using Genetic Programming	120
<i>Fenglin Yuan, Tim Mueller</i>	
(142j) Machine Learning with Structural Fingerprints of Local Particle Environments	121
<i>Matthew Spellings, Sharon C. Glotzer</i>	
(142k) Using Semi-Supervised Machine Learning to Map the Phase Diagrams of Open Materials Data Sets	122
<i>Jason Hattrick-Simpers, Jonathan Kenneth Bunn, Jianjun Hu</i>	
(150a) Sustainability Concepts in the Food-Energy-Water Nexus: Chemical Engineering Perspective	123
<i>Tapas Das, Heriberto Cabezas, Selma Mededovic Thagard</i>	
(150b) Optimizing Spatio-Temporal Sensor Placement for Nutrient Monitoring: Algorithmic Framework	124
<i>Kinnar Sen, Urmila M. Diwekar</i>	
(150c) Bandwidth Study on Energy Use and Potential Energy Saving Opportunities in Manufacturing Food and Beverages	125
<i>Caroline Kramer, Joe Cresko</i>	
(150d) Insight-Based Design of Local Integrated Systems for Food, Energy and Water	137
<i>Melissa Leung Pah Hang, Elias Martinez Hernandez, Matthew Leach, Aidong Yang</i>	
(150e) Recovering Runoff Particulate-Bound Phosphorus Via Fungal Bioextraction	138
<i>Andro Mondala, Shaun Shields, Katie Gaviglio, Jerico Alcantara, Stephen Kaczmarek, Andrew Tangonan</i>	
(150f) Preliminary Study on Detroit's Urban Food-Energy-Water (FEW) Nexus	139
<i>Sai Liang, Qiaoting Zhao, Guiyuan Xue, Ming Xu, Jeremiah Johnson, Joshua Newell, Nancy Love, Glen Daigger, Shelie Miller</i>	
(158a) Closed-Loop Scheduling: Major Considerations, Paradoxes and Remedies	140
<i>Dhruv Gupta, Christos T. Maravelias</i>	
(158b) Integration of Scheduling and Control Under Process Uncertainties	143
<i>Lisia S Dias, Jinjun Zhuge, Marianthi Ieraperitrou</i>	
(158c) A Framework for Integration of Design, Scheduling and Control for Chemical Processes Under Disturbances	144
<i>Robert Koller, Luis A. Ricardez-Sandoval</i>	
(158d) Design, Scheduling and Control: A Simultaneous Approach By Multi-Parametric Programming	145
<i>Nikolaos A. Dangelakis, Baris Burnak, Efstratios N. Pistikopoulos</i>	
(158e) Coordinating Production Scheduling and Process Operation Via Economic Model Predictive Control	148
<i>Anas Alanqar, Helen Durand, Fahad Albalawi, Panagiotis D. Christofides</i>	
(158f) Travelling Salesman Problem (TSP) Based Integration of Planning, Scheduling and Control for Continuous Processes	149
<i>Vassilis M. Charitopoulos, Lazaros G. Papageorgiou, Vivek Dua</i>	
(158g) Optimal Scheduling of Advanced Energy Plants with CO2 Capture	150
<i>Temitayo Bankole, Dustin D. Jones, Debangsu Bhattacharyya, Richard Turton, Stephen Zitney</i>	
(158h) Optimal Design and Control of a Catalytic Distillation Column. Case Study: Ethyl Tert-Butyl Ether (ETBE) Synthesis Column	151
<i>David E. Bernal, Jorge Mario Gómez</i>	
(177a) A Novel and Systematic Method for Process Intensification	154
<i>Jianping Li, Salih E. Demirel, M. M. Faruque Hasan</i>	
(177b) High-Resolution Process Design: Flowsheet Optimization with Embedded High Fidelity Unit Models	155
<i>Richard Pattison, Michael Baldea</i>	

(177c) Process Intensification of Multicomponent Distillation Configurations Using Minimum Additional Number of Heat and Mass Integration Sections.....	156
<i>Zheyu Jiang, Gautham Madenoor Ramapriya, Radhakrishna Tumbalam Gooty, Mohit Tawarmalani, Rakesh Agrawal</i>	
(177d) Novel Optimization-Based Approach for Process Design and Intensification of High-Dimensional Modular Systems.....	157
<i>Juan C. Carrasco, Fernando V. Lima</i>	
(177e) Towards Optimal and Sustainable Operation of Separation Processes: The Computational Approach.....	158
<i>Maria M. Papathanasiou, A. Mantalaris, Efstratios N. Pistikopoulos</i>	
(177f) Multi-Scale Computer Aided Synthesis–Design–Intensification Method for Sustainable Hybrid Solutions.....	159
<i>Anjan Kumar Tula, Nipun Garg, John M. Woodley, Rafiqul Gani, Bridgette Befort</i>	
(177g) Microwave Assisted Crystallization: Intensification of Direct Nucleation Control.....	160
<i>Rohit Kacker, Herman J. M. Kramer</i>	
(177h) A Systems Approach for the Development of Osn Membrane Cascades.....	161
<i>Vincentius Surya Kurnia Adi, Marcus Cook, Ludmila G. Peeva, Andrew G. Livingston, Benoît Chachuat</i>	
(181a) Solution Strategies for the Dynamic Warehouse Location Under Discrete Transportation Costs.....	162
<i>Braulio Brinaud, Matt Bassett, Anshul Agarwal, John Wassick, Ignacio Grossmann</i>	
(181b) Multiscale Production Routing in Multicommodity Supply Chains with Complex Production Facilities.....	163
<i>Qi Zhang, Arul Sundaramoorthy, Ignacio E. Grossmann, Jose M. Pinto</i>	
(181c) Supply Chain Planning and Scheduling Approach for Multiproduct Multistage Continuous Plants Under Uncertainty.....	164
<i>Adrian M. Aguirre, Songsong Liu, Lazaros G. Papageorgiou</i>	
(181d) Safety Stocks Revisited: Terminal Constraints for Closed-Loop Scheduling.....	165
<i>Yachao Dong, Christos T. Maravelias</i>	
(181e) Adaptive Robust Optimization for Tactical-Level Distribution Problems Under Customer Order Uncertainty.....	166
<i>Anirudh Subramanyam, Frank Mufalli, Jose M. Pinto, Chrysanthos E. Gounaris</i>	
(181f) Optimal Integrated Water Management and Shale Gas Supply Chain Planning Under Uncertainty.....	167
<i>Omar J. Guerra, Andrés Joaquín Calderon Vergara, Lazaros G. Papageorgiou, Gintaras V. Reklaitis</i>	
(181g) Surrogate-Based Derivative Free Optimization of a Multi-Enterprise Supply Chain.....	168
<i>Nihar Sahay, Lisia S Dias, Marianthi G. Ierapetritou</i>	
(181h) A Leader-Follower Game-Based Life Cycle Optimization Framework and Shale Gas Supply Chain Application.....	169
<i>Jiyao Gao, Fengqi You</i>	
(189c) Simulation of Propane Dehydrogenation (Catofin) Process.....	172
<i>Byeonggil Lyu, Il Moon</i>	
(189d) Product Dynamic Transitions Using a Derivative-Free Optimization Trust-Region Approach.....	174
<i>Antonio Flores-Tlacuahuac, Israel Negrellos</i>	
(190j) Advanced Modeling of Tissue:Blood Partition Coefficients for Industrial Chemicals.....	175
<i>Krystalia Papadaki, Spyros Karakitsios, Dimosthenis Sarigiannis</i>	
(245f) Optimization of Dynamic Systems Including Ordinary and Fractional Differential Equations.....	176
<i>Vicente Rico-Ramirez, Julio C. Barrera-Martinez, Edgar O. Castrejon-Gonzalez, Urmila M. Diwekar</i>	
(188l) Thin Film Deposition Using Rarefied Gas Jet.....	178
<i>Sahadev Pradhan</i>	
(249f) Non-Convex MINLP for Utility Optimization.....	183
<i>Rajkumar Vedam, Detong Zhang, Puri Tanartkit, Gareth Hillier, Sankararao Boddupalli, Mallikarjun Lavate, Manju Murali</i>	
(249z) Novel Sampling Technique for High Dimensionalstochastic Optimization/Stochastic Programmingproblems.....	187
<i>Nishant Dige, Urmila M. Diwekar</i>	
(249ab) Monte Carlo Simulation-Based Method for Process Performance Assessment in Sterile Manufacturing of Biopharmaceuticals.....	188
<i>Gioele Casola, Christian Siegmund, Markus Matern, Hirokazu Sugiyama</i>	
(189a) Modeling and Optimization of Industrial Ammonia Synthesis Process.....	189
<i>Stanislav Ivanov, Ajay K. Ray</i>	
(249g) A New Proactive Scheduling Methodology for Front-End Crude Oil and Refinery Operations Under Uncertainty of Shipping Delay.....	196
<i>Jialin Xu, Qiang Xu</i>	
(249j) A Generic MILP Modelling Framework for the Systematic Design of Lignocellulosic Biorefining Supply Chains.....	197
<i>Anna Panteli, Sara Giarola, Nilay Shah</i>	
(249h) Application of an Artificial Bee Colony Algorithm for Constrained Optimization Problems.....	200
<i>Matthew Hartenstein, Kyle Camarda</i>	
(189e) Infrastructure Maintenance and Inspection Scheduling with a Time-Variant Transition Probability Under a State Observation Uncertainty.....	201
<i>Jong Woo Kim, Jong Min Lee</i>	
(189f) Real-Time Proactive-Reactive Scheduling Under Uncertainty Using Approximate Dynamic Programming.....	203
<i>Go Bong Choi, Jong Min Lee</i>	
(189g) Performance and Dynamic Behavior of Shell Entrained-Flow Gasifier By Coals with Different Moisture and Rank in a 300 MW Integrated Gasification Combined Cycle (IGCC) Power Plant.....	205
<i>Youngsan Ju, Hyeon-Hui Lee, Min Oh, Chang-Ha Lee</i>	
(249m) Understanding Rare Safety and Reliability Events Using Transition Path Sampling.....	207
<i>Ian Moskowitz, Warren D. Seider, Amish Patel, Jeffrey E. Arbogast, Ulku G. Oktem</i>	

(189h) Chance-Constrained MINLP Optimization for the Process Synthesis of the Oxidative Coupling of Methane	208
<i>Erik Esche, David Müller, Günter Wozny, Jens-Uwe Repke</i>	
(249w) Health-Aware Operation of a Subsea Gas Compression Station Under Uncertain Operating Conditions	209
<i>Adriaen Verheyleweghen, Johannes Jäschke</i>	
(249k) Optimal Grade Transitions for a Propylene Polymerization Loop Reactor	210
<i>Maria Giuliana Fontanelli Torraga, Reinaldo Giucidi</i>	
(189i) Dynamic Global Sensitivity Analysis on Wastewater Stabilization Pond Networks	211
<i>M. Paz Ochoa, Vanina Estrada, Patricia M. Hoch</i>	
(189j) Optimization of a Dual PSA Process for the Separation of Mixture Gas Consisting of Methane and Carbon Dioxide	212
<i>Seungnam Kim, Daeho Ko, Il Moon</i>	
(249s) Optimal Decision-Making of Decentralized Multi-Participant Multi-Period Supply Chains Under Uncertainty	214
<i>Kefah Hjaila, Luis Puigjaner, Antonio España</i>	
(189l) Optimal Design of Feasible Clinical Tests for the Identification of Physiological Models of Type 1 Diabetes Mellitus	215
<i>Davide Pradella, Fabrizio Bezzo, Federico Galvanin</i>	
(190g) Advances in DEM Computing Which Improve Predictive Capability for Processes	216
<i>Howard Stamato, Aditya Vanarase, Preetanshu Pandey, Rahul Bharadwaj, Martin Hack, Lucilla Almeida, Leon W Nogueira</i>	
(245e) Travelling Traders' Exchange Problem: Stochastic Simulation and Sensitivity Analysis	218
<i>Chunbing Huang, Patrick Piccione, Federica Cattani, Federico Galvanin</i>	
(245i) Population Interaction Based on Occupation: Agriculturists and Industrialists	220
<i>Babita Verma, S. Pushpavanam</i>	
(190i) Current-Driven Dynamics of Single-Layer Epitaxial Islands on Crystalline Conducting Substrates	221
<i>Ashish Kumar, Dwaipayan Dasgupta, Dimitrios Maroudas</i>	
(245r) A Systematic Procedure for Analysis and Modification of Nonlinear Equation Sets to Enhance Convergence and Reduce Computational Effort	223
<i>Neima Brauner, Mordechai Shacham</i>	
(190h) Multivariate Data Analysis of Markers of Oxidative Stress and DNA Methylation in Children with Autism Spectrum Disorder	227
<i>Daniel P. Howson, Uwe Kruger, Stepan Melnyk, S. Jill James, Juergen Hahn</i>	
(245l) Nonlinearity Analysis of Periodically Forced Bioreactors	229
<i>Chi Zhai, Ahmet Palazoglu, Wei Sun, Zengzhi Du</i>	
(245c) Convenient Prediction of Steady State Multiplicity Patterns - Multiple Autocatalytic Reactions	232
<i>Satish J. Parulekar, Zhefu Que</i>	
(190l) Mesoscale Effects in Heat Conduction through Crystalline Solids	233
<i>Joel Christenson, Ronald J. Phillips, Robert L. Powell</i>	
(245d) A Nonlinear Programming Framework for Estimating Spatial Coupling in Disease Transmission	234
<i>Todd Zhen, Carl Laird</i>	
(245h) Scheduling and Purchasing Optimization for Olefin Cracking Complex	235
<i>Min Chen, Qiang Xu</i>	
(245u) Kinetic Parameter Estimation Including Uncertainty Under Mass Transfer Limited Conditions	236
<i>Timothy Van Daele, Krist V. Gernaey, Ingmar Nopens</i>	
(245n) A Kinetic Model of Lignin Biosynthesis in Arabidopsis thaliana for Improved Biofuel Production	237
<i>Rohit Jaini, Longyun Guo, Peng Wang, Natalia Dudareva, Clint Chapple, John A. Morgan</i>	
(245k) Minimization of Entropy Generation in Multi-Pressure Reactive Distillation Networks	238
<i>Flavio da Cruz, Vasilios Manousiouthakis</i>	
(245o) Coupled Autocatalytic Reactions: Extinction of a Species	239
<i>Aditi Khot, S. Pushpavanam</i>	
(245m) Computational Approaches in Systems Modelling for Environmental Impacts of Industries: Automating Physical Input-Output Tables (PIOTs) Via Process Modelling	241
<i>Elizabeth Wachs, Shweta Singh</i>	
(246g) Process Systems Lifecycle Management Using a Model Based Engineering Approach	242
<i>Manuel Rodriguez Hernandez, Ismael Diaz, Carlos Hernandez Corbato, Ricardo Sanz Bravo, Julia Bermejo</i>	
(246l) Comparison of Two Identification Methods for Identifying Sequential Alarms in Plant Operation Data	245
<i>Zhexing Wang, Masaru Noda</i>	
(189k) Heterogeneous Supercomputing with Multi-Scale Modeling - Towards Virtual Reality in Process Engineering	246
<i>Wei Ge</i>	
(246d) Developing a Strategy for Renewable Energy System in Process Industry with a Focus on Employing Energy Storage Systems	247
<i>Jun-Hyung Ryu</i>	
(246i) A Tree Ontology for Multi-Scale Multi-Disciplinary Process Model	248
<i>Heinz A. Preisig, Arne Tobias Elve</i>	
(246j) Data-Mining Assisted Coarse-Grained Optimization	249
<i>Dmitry Pozharskiy, Grigorios A. Pavliotis, Ioannis G. Kevrekidis</i>	
(246k) Data Analytics Applied to Reduce Hazards During Process Transitions	250
<i>M.A.K. Rasel, Yan Fang, Peyton C. Richmond</i>	
(247p) Dissimilarity-Based Fault Diagnosis through Ensemble Filtering of Informative Variables	251
<i>Chudong Tong</i>	

(190e) Systems Analysis of Ensemble of Decision Trees for Modeling and Process Control	252
<i>Zelimir Kurtanjek</i>	
(247n) Modeling Emergent Phenomena in Complex Sociotechnical Systems	263
<i>Zhizun Zhang, Venkat Venkatasubramanian</i>	
(247a) On the Robust Explicit Model Predictive Control of Hybrid Discrete-Time Linear Systems	264
<i>Richard Oberdieck, Efstratios N. Pistikopoulos, Ioana Nascu</i>	
(190a) Data Based Process Monitoring of Industrial Processes Using Multiscale Nonlinear Multivariate Statistical Methods	265
<i>Chiranjivi Botre, M. Ziyen Sheriff, Majdi Mansouri, Hazem Nounou, Mohamed Nounou, M. Nazmul Karim</i>	
(190c) Beyond Foptd Models in Tuning PI Controllers	267
<i>Yongjeh Lee, Dae Ryook Yang, Jietae Lee, Thomas F. Edgar</i>	
(247s) Hybrid Algorithms for the Design of Sensor Networks of Nonlinear Systems	268
<i>José Hernández, Mercedes Carnero, Mabel C. Sánchez</i>	
(247r) Power Plant Abnormal Condition Detection Using the Artificial Immune System Paradigm	269
<i>Ghassan Al-Sinbol, Mario Perhinschi, Debangsu Bhattacharyya</i>	
(247f) Delay-Timer Alarm Design for Uncertain Chemical Systems	270
<i>Aditya Tulsyan, Bhushan Gopaluni</i>	
(247x) Monosilane Production: Analysis and Control of a Reactive Distillation Column to Reduce Cooling Utilities	271
<i>Salvador Tututi-Avila, Nancy Medina-Herrera, Arturo Jiménez-Gutiérrez</i>	
(247q) Active Fault Detection and Isolation and False Alarm Elimination By Constrained Optimization of Built-in and Maintenance Test Conditions	272
<i>Kyle A. Palmer, William T. Hale, George M. Bolla</i>	
(247d) Exploiting Connectivity Structure for Online Selection of Primary Controlled Variables	273
<i>Temitayo Bankole, Debangsu Bhattacharyya</i>	
(190b) Control Configuration Selection Using Agglomerative Hierarchical Clustering: Graph-Theoretic Approach	274
<i>Lixia Kang, Wentao Tang, Yongzhong Liu, Prodromos Daoutidis</i>	
(247h) Steam Methane Reforming Furnace Control: Design and Implementation on a CFD Model of an Industrial Furnace	276
<i>Andres Aguirre, Anh Tran, Helen Durand, Marquis Crose, Zhe Wu, Panagiotis D. Christofides</i>	
(247m) Modeling and Control of Proppant Bank Height to Achieve Uniformity of a Hydraulic Fracturing System	277
<i>Prashanth Kumar Siddhamshetty, Seeyub Yang, Joseph Sangil Kwon</i>	
(247z) Linking Production and Utilities – A Holistic View on Plants and Energy Supply	278
<i>Florian Pöllabauer, Thomas Wallek, Gerald Bachmann</i>	
(247i) Estimation of Gasifier Wall Profile Using Measurements from a Wireless Sensor Network	279
<i>Qiao Huang, Debangsu Bhattacharyya, Ed Sabolsky</i>	
(247u) Robust Classification of Systematic Measurement Errors	280
<i>Claudia E. Llanos, Roberto J. Chávez Galletti, Mabel Sanchez, Ricardo A. Maronna</i>	
(190d) A Multivariate Data Driven Approach for Modelling the Cognitive Behaviour of Control Room Operator Using Eye Tracking	282
<i>Punitkumar Bhavsar, Babji Srinivasan, Rajagopalan Srinivasan</i>	
(190f) Improved Soft Sensors for Mixed Culture System Monitoring	283
<i>Devarshi Shah, Kyle Stone, Q. Peter He, Jin Wang</i>	
(247aa) Review of Flare Requirements and Challenges in Implementation	284
<i>Emily Manternach, Erick Mertoetomo</i>	
(247k) Modeling and Prediction of Behavior of Mammalian Cell Culture for Monoclonal Antibody Production - Dual Rate Approach	285
<i>Jingwei Gan, Satish J. Parulekar, Ali Cinar</i>	
(247e) Port Hamiltonian Approach to Modeling and Control of Coupled Chemical Reactors	286
<i>Xiaodong Xu, Stevan Dubljevic</i>	
(248d) Optimal Reactor-Separator-Network Synthesis	287
<i>Nicolas Maximilian Kaiser, Kai Sundmacher</i>	
(248m) Targeting Multi-Phase Chemical Reactor Networks in Biochemical Processes: A Superstructure Approach with a View to Innovation and Novel Development	288
<i>Georgios P. Panayiotou, Aikaterini D. Mountraki, Antonis C. Kokossis</i>	
(188b) Automatic Generation of Optimal Structure for Distillation Processes Using Stepwise VLE Description	289
<i>Hiroshi Takase, Shinji Hasebe</i>	
(248r) Design and Simulation of Biofuel Production from Pyrolysis of Brown Macroalgae	291
<i>Boris Brigljevic, J. Jay Liu, Peyman Fasahati</i>	
(248n) Computationally Efficient Evaluation of Energetically Improved Distillation Processes for the Separation of Non-Ideal Mixtures	292
<i>Thomas Waltermann, Mirko Skiborowski</i>	
(188c) An Automated Supertargeting Approach for Heating Medium System	295
<i>Pitchaimuthu Diban, Dominic Chwan Yee Foo</i>	
(248e) Systematic Process Design of Cumene Process	298
<i>Kristian R. K. Krum, Joachim Thrane, Christian B. Schandel</i>	
(248f) A Methodology for Process Debottlenecking By Process Intensification: Application to Ethylene Oxide Production	299
<i>Magda H. Barecka, Mirko Skiborowski, Andrzej Górak</i>	
(248k) Sustainable Production of Styrene By Conversion of Benzene and Ethylene Through Carbon Dioxide	302
<i>Anders Jakstrand, Tim B. Hybschmann, Julie N. Larsen, Anjan Kumar Tula</i>	

(188e) Visualization and Modeling of Chemical Processes Via Mosaic	303
<i>Bridgette Befort, Kenneth Bishop, Kyle V. Camarda, Erik Esche, Sandra Fillingner, Jens-Uwe Repke, Gregor Tolksdorf</i>	
(188i) Synthesis of Dimethyl Ether from Natural Gas: CO₂ Utilization Process	305
<i>Alessandro Duso, Júlia Rós Hafþórsdóttir, Yiyi Cao, Emmanouil Papadakis, Olivia Ana Perederic</i>	
(248ae) Integrated Biorefineries Using Ionic Liquids: Application to Macroalgae Feedstock	307
<i>Manuel Rodriguez Hernandez, Ismael Diaz</i>	
(248aa) Real-Time Dynamic Efficiency Optimization of Coal-Fired Steam Power Plants	308
<i>Chen Chen, George M. Bollas</i>	
(188k) Exergy Targeting for Complicated LNG Processes	309
<i>Donghoi Kim, Truls Gundersen</i>	
(188j) A Methodology to Generate Modular Equipment for an Equipment Database in Module-Based Plant Design	310
<i>Martin Eilermann, Christian Post, Tobias Gottschalk, Dorothea Schwarz, Stefan Leufke, Gerhard Schembecker, Christian Bramsiepe</i>	
(188f) Combined Water and Energy Integration in Industrial Processes with Restricted Connections	312
<i>Maziar Kermani, Ivan D. Kantor, François Maréchal</i>	
(188h) Comparison of Capacity Expansion Strategies for Chemical Production Plants and Consideration of Alternative Modular Reactors with a Larger Operating Window	315
<i>Heiko Radatz, Kevin Kühne, Gerhard Schembecker, Christian Bramsiepe</i>	
(248ab) Safety Evaluation of Shale Gas Monetization Processes	317
<i>Andrea Paulina Ortiz-Espinoza, Arturo Jiménez-Gutiérrez</i>	
(188g) Optimal Design of LNG Regasification Terminals	318
<i>Harsha Nagesh Rao, Zhi Xin Chew, Iftekar A. Karimi, Farooq Shamsuzzaman</i>	
(248af) A Systematic Workflow for the Design of Robust Batch Processes	319
<i>Daniel M. Casas-Orozco, Aída Luz Villa, Omar J. Guerra, Gintaras V. Reklaitis</i>	
(188a) Metabolic Network Design for Ethanol Production By <i>Synechocystis</i> sp. PCC 6803	320
<i>Romina Lasry Testa, Claudio Delpino, Vanina Estrada, Maria Soledad Diaz</i>	
(248ai) Simultaneous Optimization of Heat Exchanger Network Synthesis and Heat-Exchanger Design Using Genetic/Simulated Annealing Algorithm	322
<i>Wu Xiao, Kaifeng Wang, Xiaobin Jiang, Xiangcun Li, Xuemei Wu, Gaohong He</i>	
(190k) Production of Bioethanol from Lignocellulosic Biomass in Mexico: Evaluation on Technical Potential and the Analysis of Two Biorefinery Configurations	330
<i>Danahe Marmolejo-Correa, Edgar Vázquez-Núñez, Carlos Molina-Guerrero, J. Carlos Cárdenas, Arturo Sanchez</i>	
(248ac) Dynamic Optimization Model for a Heat and Power Plant	331
<i>Mohammed Almkhaita, Vasilios Manousiouthakis</i>	
(248w) Selection of the Optimal Operating Conditions in Fired Heaters Based on Two Phase CFD Simulations	332
<i>Danahe Marmolejo-Correa, Dionicio Jantes-Jaramillo</i>	
(266a) Monte-Carlo-Simulation-Based Optimization Methods for Copolymerization Process	333
<i>Yanman Ma, Jinzu Weng, Xi Chen, Lorenz T. Biegler</i>	
(266b) Dynamic Discrepancy Reduced Modeling: Overview and Applications	334
<i>David S. Mebane, Kujun Li, Priyadarshi Mahapatra, K. Sham Bhat, Joel D. Kress, David C. Miller</i>	
(266c) A Heterogeneous High Performance Computing Implementation of Thin Film Growth Simulation	335
<i>Xuelei Zhang, Dong Ni</i>	
(266e) Multiscale Computational Fluid Dynamics: Methodology and Application to Film Microstructure Control in PECVD	336
<i>Marquis Crose, Anh Tran, Helen Durand, Panagiotis D. Christofides</i>	
(266f) Fault Tolerant Computing through Machine Learning	337
<i>David Sroczynski, Christine Kyauk, Ioannis G. Kevrekidis, Paul Villoutreix, Joakim Anden</i>	
(266g) An Information Entropy Based Consistency Index for Evaluating the Performance of Variable Selection Methods	338
<i>Qinghua He</i>	
(266h) Parallel Solution of Parameter Estimation Problem for Polymer Models Using Multiple Grade Transition Curves	339
<i>Francisco Trespalacios, Thomas A. Badgwell</i>	
(290a) Design of Multi-Actor Distributed Processing Systems: A Game-Theoretical Approach	340
<i>Ana I. Torres, George Stephanopoulos</i>	
(290b) Optimization of Reverse Water-Gas Shift Chemical Looping for Continuous Production of Syngas from CO₂	341
<i>Marcus Wenzel, Liisa Rihko-Struckmann, Kai Sundmacher</i>	
(290c) Model-Based Comparison of Novel Hollow-Fibre Sorbent Adsorber to Packed Bed Process for Dilute Gas Streams	342
<i>Trisha Sen, Héctor Octavio Rubiera Landa, Jayashree Kalyanaraman, Yoshiaki Kawajiri, Matthew J. Realff</i>	
(290d) Profitability and Risk in Conceptual Plant Design: Dealing with Key Financial Parameters Rigorously and Simultaneously	343
<i>Duncan A. Mellichamp</i>	
(290e) Characterization and Optimal Site Matching of Wind Turbine: Effects on the Economics of Synthetic Methane Production	344
<i>Verónica de la Cruz, Mariano Martin</i>	
(290f) Multi-Objective Optimization of Biorefinery and Uncertainty Analysis	345
<i>Shivom Sharma, Ayse Dilan Celebi, François Maréchal</i>	

(290g) Development of a Semantically-Enabled Model-Sharing Biorefinery Platform	346
<i>Eirini Sioukrou, Filipoinin Lykokanellos, Antonis C. Kokossis</i>	
(290h) Optimal Production of Power in a Combined Cycle from Manure Based Biogas	347
<i>Erick León, Mariano Martín</i>	
(309a) A State-Space Formulation for Autocovariance-Based Plant-Model Mismatch Estimation in Model Predictive Control	348
<i>Jodie Simkoff, Siyun Wang, Michael Baldea, Leo H. Chiang, Ivan Castillo, Rahul Bindlish, David Stanley</i>	
(309b) Development of an Integrated Framework for Stochastic Model Predictive Control with Moving Horizon Estimation	349
<i>Bruno F. Santoro, Fernando V. Lima</i>	
(309c) Nonlinear Model Predictive Control with Explicit Performance Specification	350
<i>Masoud Kheradmandi, Prashant Mhaskar</i>	
(309d) Optimization-Based Event-Triggered Predictive Control of Process Systems with Control and Communication Constraints	351
<i>Da Xue, Nael H. El-Farra</i>	
(309e) Output-Feedback Predictive Control for Stochastic Nonlinear Systems	354
<i>Vinay Bavdekar, Ali Mesbah</i>	
(309f) Strategies Towards the Robust Multi-Parametric Control of Continuous-Time Systems	355
<i>Muxin Sun, Mario E. Villanueva, Benoit Chachuat, Efstratios N. Pistikopoulos</i>	
(309g) On the Moment-Based Robust MPC Formulations	358
<i>Muhammed B. Saltik, Leyla Özkan, Jobert H.A. Ludlage, Siep Weiland, Paul M.J. Van den Hof</i>	
(309h) Robust Optimization Approximation of Chance Constrained Model Predictive Control	361
<i>Wenhan Shen, Zukui Li, Biao Huang, Fraser Forbes</i>	
(314a) Recent Advances in the BARON Project	362
<i>Yash Puranik, Mustafa Kilinc, Nick Sahinidis</i>	
(314b) Using Functional Programming to Recognize Named Structure in an Optimization Problem: Application to Pooling	363
<i>Francesco Ceccon, Ruth Misener</i>	
(314c) Tools and Workflows in the Design of Urban Energy Systems	366
<i>Kamal Kuriyan, Nilay Shah</i>	
(314d) PlasmO: Platform for Scalable Modeling and Optimization	367
<i>Yankai Cao, Jordan Jalving, Kibaek Kim, Victor M. Zavala</i>	
(314e) Analytics Framework and Infrastructure - Integrating Big-Data Cloud Technologies with First-Principle Modeling	368
<i>Apurva P. Samudra, Alexander B. Smith, Bijan Sayyar-Rodsari</i>	
(314f) Recent Developments in Pyomo	369
<i>John Siirola, William E. Hart, Jean-Paul Watson</i>	
(314g) Thermodynamic Consistency-Based Validation Approach for Equation of State Methods in Process Simulators	370
<i>Seiya Hirohama, Prasad Narasimhan, Francisco Braña-Mulero, Nevin Gerek, David Bluck</i>	
(319a) Managing Trade-Offs Between Food, Renewable Energy and Ecosystem Services	375
<i>Rebecca Hanes, Varsha Gopalakrishnan, Bhavik R. Bakshi</i>	
(319b) Efficient Solar Thermal Hydrogen, Electricity and Fresh Water Coproduction Process Synthesis	376
<i>Emre Gençer, Rakesh Agrawal</i>	
(319c) Food-Energy-Water Nexus: Modeling Energy and GHG Emissions of Water Embodied in U.S. Domestic Food Transfers	377
<i>Nemi Vora, Apurva Shah, Vikas Khanna</i>	
(319d) Water Footprint of Hydrotreated Renewable Jet Fuel Produced through Rapeseed Rotation with Wheat and Other Crops in North Dakota	378
<i>Rui Shi, David W. Archer, Suchada Ukaew, Kristin C. Lewis, David R. Shomard</i>	
(319e) NexSym – A Local Nexus Simulation System	379
<i>Elias Martinez Hernandez, Melissa Leung Pah Hang, Matthew Leach, Aidong Yang</i>	
(319f) Gibbsian Game Theory for Tragedy of the Commons Problems in Food-Energy-Water Sustainability	380
<i>Darrell Velegol</i>	
(319g) Water and Energy Systems in Sustainable City Development: Agent-Based Modelling and Resource Technology Optimization	381
<i>Xiaonan Wang, Koen H. van Dam van Dam, Charalampos Triantafyllidis, Rembrandt Koppelaar, Nilay Shah</i>	
(333a) Visualization and Analysis of Periodic Process Data	382
<i>Ray Wang, Michael Baldea, Thomas F. Edgar, Mark Nixon, Willy Wojsznis, Ricardo Dunia</i>	
(333b) Iot-Enabled Cybermanufacturing: Challenges and Possibilities	383
<i>Devarshi Shah, Austin Hancock, Anthony Skjellum, Q. Peter He, Jin Wang</i>	
(333d) An Optimization-Based Approach for Learning Simple Parametric Surrogate Models	384
<i>Zachary Wilson, Nick Sahinidis</i>	
(333e) M.R.Q.P.: Prediction of Final Batch Quality Using a Multi-Resolution Framework	385
<i>Geert Gins, Jan Van Impe, Marco Reis</i>	
(333f) Process Knowledge Discovery and Selecting Number of Non-Zero Loadings in Sparse Principal Component Analysis	388
<i>Shriram Gajjar, Murat Kulahci, Ahmet Palazoglu</i>	
(333g) Deep Reinforcement Learning Approach for Process Control	389
<i>Steven Spielberg Pon Kumar, Bhushan Gopaluni, Rohit Patwardhan, Philip Loewen</i>	

(333h) The Distribution of Online News Evaluated By Chemical Engineering and Process Control Tools	390
<i>Robert N. Grass, Wendelin J. Stark</i>	
(341a) Identifying Circadian Drug Targets for Maintained Oscillatory Precision	391
<i>John H. Abel, Francis J Doyle</i>	
(341b) A Systems-Biology Approach to Investigate the Antimicrobial Activity of Oleuropein	392
<i>Xianhua Li, Yanhong Liu, Qian Jia, Virginia LaMacchia, Kathryn O'Donoghue, Zuyi (Jacky) Huang</i>	
(341c) VEGFR1 Mediates Cell Migration through Activation of PI3K and PLC	393
<i>Jared Weddell, Princess Imoukhuede</i>	
(341d) Developing a Stochastic Model of LPS-Induced TNF-α Production in Macrophages	396
<i>Dongheon Lee, Yufang Ding, Arul Jayaraman, Joseph Sangil Kwon</i>	
(341e) Parameter Estimation for Sparse Biological Data: Glucose-Dependence of Renin-Angiotensin System in Podocytes Cells during Diabetic Kidney Disease	397
<i>Minu R. Pilvankar, Michele A. Higgins, Ashlee N. Ford Versypt</i>	
(341f) A Method for Learning a Sparse Classification Model in the Presence of Missing Data	398
<i>Kristen Severson, Brinda Monian, J. Christopher Love, Richard D. Braatz</i>	
(341g) Optimal Experiment Design for Uncertain Biological Systems	399
<i>Marc Martin-Casas, Ali Mesbah</i>	
(341h) Data-Driven Parameter Reduction in Sloppy Models	400
<i>Alexander Holiday, Antonios Zagaris, William E. Leeb, William Gear, I.G. Kevrekidis</i>	
(359a) Process Systems Engineering Beyond Chemical Plants: Signed Digraph As a Modeling Tool for Analyzing Systemic Risk in Financial Networks	401
<i>Richard Bookstaber, Paul Glasserman, Garud Iyengar, Yu Luo, Venkat Venkatasubramanian, Zhizun Zhang</i>	
(359c) Multiperiod Inventory Pinch Algorithm for Integrated Planning and Scheduling of Oil Refineries	402
<i>Pedro Castillo Castillo, Pedro M. Castro, Vladimir Mahalec</i>	
(359d) Improved Data-Driven Mathematical Modeling and Global Optimization Framework: An Application in Refinery Planning Operations	405
<i>C. Doga Demirhan, Fani Boukouvava, Kyungwon Kim, Hyeju Song, Christodoulos A. Floudas</i>	
(359e) Evaluation of Smart Manufacturing (SM) Benefits in Industrial Steam-Methane Reformers (SMR)	406
<i>Ankur Kumar, Michael Baldea, Thomas F. Edgar</i>	
(359f) Development of a High Fidelity and Reduced Order Data-Driven Model of Hydrogen Plant	407
<i>Abhinav Garg, Brandon Corbett, Prashant Mhaskar, Gangshi Hu, Jesus Flores-Cerrillo</i>	
(359g) Computation and Analysis of Optimal Operating Strategies for Air Separation Units Using High Fidelity Dynamic Models	409
<i>Yanan Cao, Christopher L. E. Swartz, Jesus Flores-Cerrillo</i>	
(374a) Tailor-Made Solvent and Process Design for the Separation of Azeotropic Mixtures	411
<i>Rafiqul Gani, Anjan Kumar Tula, Deenesh K. Babi, Marta Gonzalez Garcia</i>	
(374b) A Target Upper Bound on Reaction Selectivity Via Feinberg's Cfstr Equivalence Principle	414
<i>Jeffrey A. Frumkin, Michael F. Doherty</i>	
(374c) A Nonsmooth Inside-Out Algorithm for Robust Flash Calculations	415
<i>Harry A. J. Watson, Matias Vikse, Donghoi Kim, Truls Gundersen, Paul I. Barton</i>	
(374d) Simultaneous Chemical Process Synthesis and Heat Integration with Unknown Cold/Hot Process Streams	416
<i>Lingxun Kong, Venkatachalam Avadiappan, Kefeng Huang, Christos T. Maravelias</i>	
(374e) A Method for Minimization of Total Exergy Loss over the Complete Search Space of Regular Distillation Configurations	417
<i>Zheyu Jiang, Gautham Madenoor Ramapriya, Radhakrishna Tumbalam Gooty, Mohit Tawarmalani, Rakesh Agrawal</i>	
(374f) Shale Gas to Light Olefins: Global Optimization of an Integrated NGL Recovery, Steam Cracking, and Methane Conversion Superstructure	418
<i>Onur Onel, Alexander M. Niziolek, Christodoulos A. Floudas</i>	
(374g) An Algorithm for Integrated Molecular and Process Design: Physically-Driven Domain Reduction for Liquid-Liquid Extraction	419
<i>Smitha Gopinath, Amparo Galindo, George Jackson, Claire S. Adjiman</i>	
(374h) Optimisation-Based Design of a Heat-Integrated Crude Oil Distillation System Using Rigorous Simulation and Surrogate Models	420
<i>Dauda Ibrahim, Jie Li, Gonzalo Guillén-Gosálbez, Megan Jobson</i>	
(383a) A Neutron Scattering Study of Ion-Conduction Mechanisms in Nanocomposite Polymer Electrolytes	421
<i>Lalitha Ganapatibhotla, Janna K. Maranas</i>	
(383b) Mechanical Properties of Graphene-Polymer Nanocomposites	422
<i>Asanka Weerasinghe, Chang-Tsan Lu, Ashwin Ramasubramaniam, Dimitrios Maroudas</i>	
(383c) Probing Multiscale Structure in Aligned Nanotube-Polymer Composites	423
<i>Eric Meshot, Ngoc Bui, Kuang Jen Wu, Francesco Fornasiero</i>	
(383d) Thermal and Mechanical Property Predictions for Conjugated Polymers Using Atomistic Simulations	424
<i>Ramaswamy Ishwar Venkatanarayanan, Sitaraman Krishnan, Arvind Sreeram, Philip Yuya</i>	
(383e) Importance of Selecting Right Analytical Tools for Successful Product Development: Case Study of Single and Two Phase Polymerization Reactions	425
<i>Kishori Deshpande, Serena Stephenson, Ravi Dixit, Pradeep Jain, Praveenkumar Boopalachandran, Shawn Chen, Carlos M. Villa, Philippe Hayot, David Park</i>	
(383f) Computer Aided Design of Ionic Liquids through a New Group Contribution Approach Based on Surface Charge Density and COSMO-SAC Predictions	426
<i>Reza Farahipour, Arunprakash T. Karunanithi</i>	

(383g) Identification of Magnetic Nanoparticles to Eradicate Cancer Cells Using the Hyperthermia Approach – A Computational Search Approach	427
<i>Shounak Datta, Mario Richard Eden</i>	
(383h) Machine Learning and Natural Language Processing for Pharmaceutical Product Engineering	428
<i>Miguel Francisco Remolona, Venkat Venkatasubramanian</i>	
(390a) Algorithms for a Closed-Loop Artificial Pancreas: Challenges and Solutions Pertinent to Chemical Process Operations and Control	429
<i>B. Wayne Bequette, Faye Cameron, Nihat Baysal, Daniel P. Howsmon, Bruce Buckingham, David Maahs, Carol Levy</i>	
(390b) A Robust Hybrid Model Predictive Control Framework for Hill Curve Model-Based Systems	430
<i>Ioana Nascu, Richard Oberdieck, Efstratios N. Pistikopoulos</i>	
(390c) Stochastic Nonlinear Model Predictive Control Using Adaptive Polynomial Chaos: Application to an Atmospheric Pressure Plasma Jet	431
<i>Edward Buehler, Ali Mesbah</i>	
(390d) Proportional State-Feedback Controller Design Using MPC Structure and Carleman Approximation Method	432
<i>Negar Hashemian, Antonios Armaou</i>	
(390e) Constrained Control Lyapunov Functions: Design and Application for Nonlinear Systems	433
<i>Tyler Homer, Prashant Mhaskar</i>	
(390f) Input-Output Paring Accounting for Both Structure and Strength in Coupling	434
<i>Xunyuan Yin, Jinfeng Liu</i>	
(390g) Elucidating and Handling Valve-Induced Nonlinearity in Industrial Feedback Control Loops	435
<i>Helen Durand, Panagiotis D. Christofides</i>	
(390h) Design and Implementation of a Biologically-Inspired Optimal Control Strategy (BIO-CS) for Advanced Energy Systems	436
<i>Gaurav V. Mirlekar, Fernando V. Lima</i>	
(398a) The Mesoscopic Behavior of Stochastic Schlogl Model	437
<i>Michail Vlysidis, Yiannis N. Kaznessis</i>	
(398b) Reaction Network Analysis for Thin-Film Deposition Processes: Physical Interpretation of Reaction Invariants	438
<i>Hossein Salami, Krishnaprasath Ramakrishnan, Raymond A. Adomaitis</i>	
(398c) Inferring Gene Regulatory Networks from Single Cell Expression Data	439
<i>Nan Papili Gao, Rudiyanto Gunawan</i>	
(398d) Modeling for Complex Interactive Behaviors Among Enterococcus Faecalis Donor and Recipients in Biofilms	443
<i>Vu Tran, Arpan Bandyopadhyaya, Gary M. Dunny, Doraiswami Ramkrishna, Wei-Shou Hu</i>	
(398e) Elucidating the Meaning of Alternative Optimal Solutions in Flux Balance Analysis	444
<i>Matthew Hilliard, Q. Peter He, Jin Wang</i>	
(398f) The Impact of Resource Constraints on the Reverse Engineering of Biological Pathways	445
<i>Tyler Quarton, Eduardo Sontag, Leonidas Bleris</i>	
(398g) Interaction Network-Based Antiviral Protein Discovery	446
<i>Jason Shoemaker</i>	
(398h) Complex Traveling Wave Phenomena Mediated By the Coupling of Phosphorylation Cascades and Extracellular Diffusion in Cellular Populations	447
<i>Michal Pribyl, Vladislav Nevoral, Igor Schreiber</i>	
(425a) Global Optimization of Crude Oil Scheduling with Discrete and Continuous-Time Formulations	458
<i>Pedro M. Castro</i>	
(425b) Optimal Scheduling of a Renewable Ammonia Plant with Wind Generation Under Variable Electricity Pricing	461
<i>Andrew Allman, Prodromos Daoutidis</i>	
(425c) Discrete-Time Mixed-Integer Programming Models for Scheduling in Sequential Environments	462
<i>Hojae Lee, Andres F. Merchan, Christos T. Maravelias</i>	
(425d) Emission Considered Scheduling for Crude Unloading, Transferring, and Processing	463
<i>Jialin Xu, Jian Zhang, Qiang Xu</i>	
(425e) A Game Theoretic Framework for Strategic Production Planning	464
<i>Philip Tominac, Vladimir Mahalec</i>	
(425f) Solution Methods for Discrete-Time Formulations for Scheduling in Multi-Stage Facilities	465
<i>Andres F. Merchan, Hojae Lee, Christos T. Maravelias</i>	
(425g) Production Planning and Scheduling Integration through Multiparametric Bilevel Mixed-Integer Optimization	466
<i>Styliani Avraamidou, Nikolaos A. Diangelakis, Richard Oberdieck, Efstratios N. Pistikopoulos</i>	
(425h) Scheduling and Internet of Things - Vision or Reality?	467
<i>Iiro Harjunkoski</i>	
(426a) Nature in Engineering: Expanding the Engineering Design Space By Including Ecosystem Goods and Services	468
<i>Bhavik R. Bakshi, Varsha Gopalakrishnan, Xinyu Liu, Rebecca Hanes, Geoffrey F. Grubb</i>	
(426b) Heat-Integrated Work Exchange Network Design	471
<i>Aida Amini Rankouhi, Yinlun Huang</i>	
(426c) Discovery and Assessment of Integrated Waste Biorefinery Paths with Conventional Industry Using an Ontology Engineering Approach	472
<i>Foteini Barla, Antonis C. Kokossis, Filipoimin Lykokanellos</i>	

(426d) Ionic Liquid Design and Sustainable Process Simulation for Decarbonization of Shale Gas and Gas Separations	473
<i>Xinyan Liu, Ying Huang, Yongsheng Zhao, Xiangping Zhang, Suojiang Zhang, Rafiqul Gani</i>	
(426e) Developing Rapid Life Cycle Inventories for Chemical Processes	474
<i>Raymond L. Smith, Gerardo J. Ruiz-Mercado, David E. Meyer, Michael A. Gonzalez, John P. Abraham, William M. Barrett</i>	
(426f) Sustainable Integration of Refineries and Biorefineries with Forest Plantations to Reduce Emissions	475
<i>Aurora de Fatima Sanchez-Bautista, José Ezequiel Santibañez-Aguilar, José María Ponce-Ortega</i>	
(430a) A Hybrid Framework for Process Synthesis-Design: Application to Biorefineries	476
<i>Maria-Ona Bertran, Ana-Sofia Sanchez-Arcilla, John M. Woodley, Rafiqul Gani</i>	
(430b) A New Heat Integration Model for Simultaneous Utility and Total Heat Exchanger Area Targeting	477
<i>Lingxun Kong, Yaqing Wu, Christos T. Maravelias</i>	
(430c) Optimal Composition of Biogas for Methanol Production Via Dry Reforming	478
<i>Borja Hernández, Mariano Martín</i>	
(430d) Production of Benzene, Toluene, and Xylenes from Natural Gas Via Methanol: A Process Synthesis and Global Optimization Approach	479
<i>Alexander M. Niziolek, Onur Onel, Christodoulos A. Floudas</i>	
(430e) Extensive Sensitivity Analysis and Stochastic Global Optimization for Renewable Energy Businesses Under Operational Level Uncertainties	480
<i>Santiago D. Salas, Aryan Geraili, Jose A. Romagnoli</i>	
(430f) Toward a Unified Method for Process Design, Integration and Intensification	481
<i>Salih E. Demirel, Jianping Li, M. M. Faruque Hasan</i>	
(430g) Work and Heat Exchange Networks - From Thermodynamic Insight to Optimization Based Design Procedures	482
<i>Truls Gundersen, Chao Fu</i>	
(430h) Analysis, Synthesis and Optimization of Multiple-Effect Evaporation Systems Using Mathematical Programming	485
<i>Elvis Ahmetovic, Midhat Suljkanovic, Zdravko Kravanja, François Maréchal, Nidret Ibric, Nesib Mustafic, Maziar Kermani, Milos Bogataj</i>	
(455a) Process to Planet Framework for Sustainable Design: Systematic Approach for Developing a Multiscale Model and for Multiobjective Optimization	486
<i>Tapajyoti Ghosh, Bhavik R. Bakshi</i>	
(455b) Application of a Shale Environmental Footprint Optimization Tool to Enhance Operational Excellence – A Case Study of Selecting Process Fuels with Lower Cost and Less Potential for Impacts to Power Chevron Operations	489
<i>Hong Jin, Janet Peargin, Abby Kirchofer, Oliver Schuller</i>	
(455c) GHG Life Cycle Assessment for the United Arab Emirates Electricity Sector Combining Optimization and Simulation Tools	490
<i>Alberto Betancourt-Torcat, Mohammed Alkatheri, Ali Almansoori</i>	
(455d) Data Envelopment Analysis Coupled with Thermodynamic and Life Cycle Assessment Metrics for Solvent Screening: Application to CO2 Capture	497
<i>Phantisa Limleamthong, Gonzalo Guillén-Gosálbez, María González Miquel, Stavros Papadokostantakis</i>	
(455e) Using Multiobjective Optimization and Life Cycle Assessment for the Design of More Sustainable National and International Energy Systems	498
<i>Nagore Sabio, Kathrin Volkart, Martin Densing, Neil Strachan</i>	
(455f) Life Cycle Assessment and Multiobjective Optimization in a Natural Gas Based Petrochemical Complex	501
<i>Fabio Antonio González Castaño, Jose Alberto Bandoni, Maria Soledad Diaz</i>	
(456a) Uncertainty Considerations for Surrogate Functions for Constrained Grey-Box Optimization	502
<i>Fani Boukouvala, Yannis A. Guzman, Christodoulos A. Floudas</i>	
(456b) Optimization of Constrained and Multidimensional Black-Box Problems Using Convex Hull Approximation and Single-Dimension Surrogate Model	503
<i>Ishan Bajaj, M. M. Faruque Hasan</i>	
(456c) Nonlinear Robust Optimization for Process Design and Operations	505
<i>Yuan Yuan, Zukui Li, Biao Huang</i>	
(456d) Differentiable McCormick Relaxations for Global Optimization	506
<i>Kamil A. Khan, Harry A. J. Watson, Paul I. Barton</i>	
(456e) Sensitivity Analysis of Uncertain Dynamic Systems Using Set-Valued Integration with Application to Complete-Search Optimization	507
<i>Nikola D. Peric, Mario E. Villanueva, Benoit Chachuat</i>	
(456f) A Novel Deterministic Global Optimization Algorithm and Its Application to Oil Refinery Planning	508
<i>Pedro Castillo Castillo, Pedro M. Castro, Vladimir Mahalec</i>	
(456g) The Cluster Problem in Constrained Global Optimization	511
<i>Rohit Kannan, Paul I. Barton</i>	
(456h) A Framework for Multi-Stakeholder Decision-Making and Conflict Resolution	512
<i>Alexander W. Dowling, Gerardo J. Ruiz-Mercado, Victor M. Zavala</i>	
(471a) Systematic Process Design Strategies for Efficient and Synergistic Integration of Solar Thermal Hydrogen, Electricity and Fresh Water Production Processes	513
<i>Emre Gençer, Mohit Tawarmalani, Rakesh Agrawal</i>	
(471b) Ideas As a Process Intensification Tool with Application to Natural Gas Reforming Based Hydrogen Production	514
<i>Patricia Pichardo, Vasilios Manousiouthakis</i>	

(471c) Optimal Design of Integrated Upgrading Plant and Utility System for the Oil Sands Industry	515
<i>Hossein Shahandeh, Zukui Li</i>	
(471d) Design and Operation of a 10 MWe Supercritical CO₂ Recompression Brayton Power Cycle	516
<i>Stephen E. Zitney, Eric A. Liese</i>	
(471e) Integrated Thermochemical Process for Optimal Co-Production of Liquid Fuels and Chemicals	517
<i>Zhihong Yuan, Mario Richard Eden</i>	
(471f) Design and Optimization of Integrated Carbon Capture and Conversion with Natural Gas to Produce Syngas	518
<i>Shachit S. Iyer, Priyadarshini Balasubramanian, Ishan Bajaj, M. M. Faruque Hasan</i>	
(471g) Optimal Design and Operation of a Semi-Closed Oxy-Combustion Combined Cycle Power Plant	519
<i>Holger Teichgräber, Adam Brandt</i>	
(471h) Natural Gas to Liquids, Olefins, and Aromatics Under Uncertainty in Feedstock and Product Prices	520
<i>Alexander M. Niziolek, Onur Onel, Logan R. Matthews, Yannis A. Guzman, Christodoulos A. Floudas</i>	
(479a) Improving Industrial Polyethylene Production Via Data Analysis	521
<i>Mohsen Nikkhoo, Job D. Guzman, Francesco Bertola</i>	
(479b) Parsimonious Modeling Approaches for Batch Process Analysis	522
<i>Ricardo Rendall, Bo Lu, Ivan Castillo, Swee-Teng Chin, Leo H. Chiang, Marco Reis</i>	
(479c) Nonlinear SVM-Based Feature Selection for Fault Detection and Diagnosis of Continuous Processes	523
<i>Chris A. Kieslich, Yannis A. Guzman, Melis Onel, Christodoulos A. Floudas</i>	
(479e) Data Management and Integration for Continuous Pharmaceutical Manufacturing	524
<i>Ravendra Singh, Huiyi Cao, Srinivas Mushnoori, Barry Higgins, Chandrasekhar Kollipara, Adam Fermier, Doug Hausner, Shantenu Jha, Marianthi Ieraperitrou, Rohit Ramachandran</i>	
(479f) Sipat 5.0 – The Next Generation of PAT Data Management	525
<i>Kjell Francois, Pamela Docherty</i>	
(479g) Enabling Data Integration in Pharmaceutical Digital Supply Chains Using Ontologies	526
<i>Nikolaos Trokanas, Jagjit Singh Srari</i>	
(479h) An Ontology-Driven Knowledge Management Framework for Public Health	527
<i>Zhiyun Zhang, Mila Gonzalez, Venkat Venkatasubramanian</i>	
(488a) Economic Nonlinear Model Predictive Control of an Integrated Solid-Sorbent Carbon Capture System	528
<i>Mingchao Yu, Lorenz T. Biegler</i>	
(488b) State Estimation of Energy Integrated Systems with Time-Scale Multiplicity	529
<i>Franklin D. Rincón, Fernando V. Lima</i>	
(488c) Biomass-Based Production of Benzene, Toluene, and Xylenes Via Methanol: Process Synthesis and Deterministic Global Optimization	530
<i>Alexander M. Niziolek, Onur Onel, Yannis A. Guzman, Christodoulos A. Floudas</i>	
(488d) A Supervisory Control Framework for Fault-Tolerant Dispatch of Distributed Energy Resources	531
<i>James Allen, Nael H. El-Farra</i>	
(488e) Grid-Relevant Demand Response Modeling of Chemical Processes	534
<i>Joannah Otashu, Cara Touretzky, Michael Baldea</i>	
(488f) Model-Guided Optimization of Polymer-Electrolyte Dye Sensitized Solar Cells	535
<i>Yuriy Y. Smolin, Kenneth K.S. Lau, Masoud Soroush</i>	
(488g) A Model-Based Feedback Optimization Method for Solar Dish Facets Alignment	536
<i>Zhenyu Yi, Dong Ni</i>	
(488h) Model Predictive Control of Solar Thermal System with Borehole Seasonal Storage	537
<i>Qingqing Xu, Stevan Dubljevic</i>	
(489b) Sustainability Assessment and Life Cycle Inventories of Bio-Based Chemicals Using Performance Indicators	538
<i>Gerardo J. Ruiz-Mercado, Michael A. Gonzalez, Raymond L. Smith</i>	
(489c) Modeling for the Life Cycle Assessment of Dry Reforming Technology – Challenges and Lesson Learnt	539
<i>Alessandra R. Carreon, Shaik Afzal, Nimir O. Elbashir, Mohamedsufiyan Challiwala, Mahmoud El-Halwagi</i>	
(489d) Performance Analysis of Chemical-Looping Fixed Bed Reactors Integrated in Combined Cycle Power Plants	540
<i>Chen Chen, Lu Han, George M. Bollas</i>	
(489e) Chemical Looping Carbon Neutral and Carbon Negative Schemes for a Gas to Liquid Fuel Facility Thermodynamic, Techno-Economic and Experimental Analysis	541
<i>Mandar Kathe, L.-S. Fan, William Wang, Abbey Empfield, Elena Blair, Charlie Fryer, Peter Sandvik</i>	
(489f) Techno-Economic Analysis of Metal-Organic Framework Materials for Onboard, Light-Duty Vehicle Hydrogen and Natural Gas Storage	542
<i>Daniel DeSantis, Cassidy Houchins, Brian D. James, Jarad A. Mason, Michael Veenstra, Jeffrey R. Long</i>	
(514a) Global Optimization Algorithm for Miqcps Featuring Spatial Branch-and-Bound and Multiparametric Disaggregation	543
<i>Pedro M. Castro</i>	
(514b) Multi-Parametric Quadratic Programming: Past, Present and Future	546
<i>Richard Oberdieck, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos</i>	
(514c) Multiparametric Programming Based Algorithms for Bilevel Mixed-Integer Linear and Quadratic Programming Problems	547
<i>Styliani Avraamidou, Richard Oberdieck, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos</i>	
(514d) Deterministic Global Optimization of Large-Scale Pooling Problems Via Topological Branch-and-Bound	548
<i>Radu Baltean-Lugojan, Ruth Misener</i>	

(514e) Solving Mpcps with IPOPT	549
<i>Wei Wan, Lorenz T. Biegler</i>	
(514f) Feasibility Pump for Solving Convex MINLP Problems with Dicopt	550
<i>David E. Bernal, Stefan Vigerske, Francisco Trespalacios, Ignacio E. Grossmann</i>	
(514g) Rigorous Surrogate-Based Optimization Strategies That Integrate Glass Box/Black Box Process Models	551
<i>John P. Eason, Lorenz T. Biegler</i>	
(514h) Capacity Planning of Industrial Gas Plants with Rational Markets Under Demand Uncertainty	552
<i>Anvitha Kandiraju, Pablo Garcia-Herreros, Ignacio E. Grossmann, Pratik Misra, Erdem Arslan, Sanjay Mehta</i>	
(527a) Implementing Robust Vapor-Liquid Equilibrium Calculations in Nonsmooth Multi-Stream Heat Exchanger Models	553
<i>Matias Vikse, Harry A. J. Watson, Truls Gundersen, Paul I. Barton</i>	
(527b) Shared and Practical Approach to Conserve Utilities in Eco-Industrial Parks	554
<i>Sajitha K. Nair, Yingjian Guo, Ushnik Mukherjee, Iftekar A. Karimi, Ali Elkamel</i>	
(527c) Optimal Design and Operation of Integrated Multi-Vector Energy Networks	557
<i>Sheila Samsatli, Nouri J. Samsatli</i>	
(527d) Simultaneous Optimization of Design and Operation Strategies for CHP Systems	558
<i>Abigail Ondeck, Michael Baldea, Thomas F. Edgar</i>	
(527e) Exploiting Dynamic Flexibility to Enable Participation in Multi-Scale Electricity Markets	559
<i>Alexander W. Dowling, Ranjeet Kumar, Victor M. Zavala</i>	
(527f) A Rolling Horizon Scenario-Based Approach for Smart House Management Under Uncertainty	560
<i>Javier Silvente, Georgios M. Kopanos, Vivek Dua, Lazaros G. Papageorgiou</i>	
(527g) Optimization Models for Shale Gas Well Refracture Treatments	561
<i>Markus G. Drouven, Diego C. Cafaro, Ignacio E. Grossmann</i>	
(527h) A Composite-Curve-Based Biomass Procurement Planning Approach	563
<i>Wenzhao (Tony) Wu, Daniel Kurniawan, Wenbo Zhu, Christos T. Maravelias</i>	
(540a) CFD Modeling and Computation for an Industrial Steam Methane Reforming Furnace	566
<i>Andres Aguirre, Anh Tran, Helen Durand, Marquis Crose, Panagiotis D. Christofides</i>	
(540b) Toward Optimal NGL Conversion to Olefins: Advances in Steam Cracking Optimization	567
<i>Onur Onel, Alexander M. Niziolek, Christodoulos A. Floudas</i>	
(540c) Decarbonization of Electricity Grids: A Multi-Scale Challenge	568
<i>Mahdi Sharifzadeh, Nilay Shah</i>	
(540d) Efficient Global Optimization for a Mixed AC-DC Power Distribution System	569
<i>Dan Li, Xiang Li</i>	
(540e) Data-Driven Modeling of Gas Leakage from Shale Natural Gas Wells	570
<i>Shobhit Misra, Michael Nikolaou</i>	
(540f) The Simulation of an Industrial Wet Flue Gas Desulfurization Absorber	571
<i>Raymond Everson, Arif Arif, David Branken, Hein Neomagus, Samrana Arif</i>	
(540g) Modeling Chemotactic Bacterial Transport in Physically Homogeneous Groundwater Systems Containing Distributed Contaminant Sources	572
<i>Joanna S. T. Adadevoh, Roseanne M. Ford</i>	
(540h) Analytical Calculation of Laminar Flow Reactor Effluent Concentrations Without the Necessity of a CFD Approach	573
<i>Vasilios Manousiouthakis, Nicholas Margull</i>	
(552a) Active Fault Diagnosis for Stochastic Nonlinear Systems	574
<i>Memia Fendri, Ali Mesbah</i>	
(552b) Sparse Nonlinear Features Based Locally Weighted Kernel Partial Least Squares for Virtual Sensing of Nonlinear Time-Varying Processes	575
<i>Ximin Zhang, Manabu Kano</i>	
(552c) Fault Detection and Isolation and Optimal Parking for HVAC Systems	579
<i>Hadi Shahnazari, Craig McDonald, Prashant Mhaskar, John House, Tim Salisbury</i>	
(552d) Pipe-Flows Leak Detection, Size Estimation and Localization	582
<i>Xiaodong Xu, Stevan Djubljevic</i>	
(552e) Model-Based Fault Detection for Nonlinear Process Systems	583
<i>Ernie Che Mid, Vivek Dua</i>	
(552f) Fault Estimation and Performance-Based Accommodation in Multi-Rate Sampled-Data Process Systems	584
<i>James Allen, Nael H. El-Farra</i>	
(552g) Multi-Rate Reduced-Order Observer Design with Application to Monitoring of Gas-Phase Polyethylene Reactors	587
<i>Chen Ling, Costas Kravaris</i>	
(552h) Comparison of Stochastic Fault Detection and Diagnosis Algorithms for Nonlinear Chemical Processes	588
<i>Yuncheng Du, Hector M. Budman, Thomas A. Duever</i>	
(580a) An Ontology Supported Integration Framework for Models and Data in Biorefining	589
<i>Linsy Koo, Nikolaos Trokanas, Franjo Cecelja</i>	
(580b) A Biorefinery Boutique Made in Switzerland	590
<i>Merten Morales, Michael Ehrenstein, Johanna Dragan, Sudharsan Ravi, Stavros Papadokostantakis, Elisabet Capón-García, Konrad Hungerbühler</i>	
(580c) New Short-Cut Tools for Early-Stage Investment Evaluation of Biorefineries	591
<i>Mirela Tsagkari, Jean-Luc Couturier, Antonis C. Kokossis, Jean-Luc Dubois</i>	

(580d) Global Sensitivity Analysis of Economic Assessment of Early Stage Process Design: The Case of the Glycerol Biorefinery	592
<i>Gürkan Sin, Carina Gargalo, Ana Isabel Carvalho, Krist V. Gernaey</i>	
(580e) General Bio-Separation Superstructure Optimization Framework	593
<i>Wenzhao (Tony) Wu, Christos T. Maravelias, Kirti Yenkie</i>	
(580f) Technoeconomic Study of AB Synthesis for Biobutanol Production	596
<i>Santiago Malmierca, Rebeca Díez, Ana I Paniagua, Mariano Martín</i>	
(580g) Effect of Market and Technical Parameter Uncertainties on the Optimal Design of Integrated Biorefineries	597
<i>Aryan Geraili, Jose Romagnoli</i>	
(582a) Centroidal Voronoi Tessellation Based Model Order Reduction for a Moving Boundary Problem: Application to a Hydraulic Fracturing System	598
<i>Abhinav Narasingam, Joseph Sangil Kwon</i>	
(582b) Output Feedback Control of Transport-Reaction Processes with Unknown Parameters Using Adaptive Model Reduction with Minimum Feedback Information	599
<i>Davood Babaei Pourkargar, Antonios Armaou</i>	
(582c) Output Regulation for Boundary Controlled Linear Coupled Hyperbolic Pides: Application to a Parallel-Flow Heat Exchanger System	600
<i>Xiaodong Xu, Stevan Dubljevic</i>	
(582d) A Novel Approach for Mechanistic Modeling and Simulation of Convection-Diffusion-Reaction Systems: Application to Nanoparticle Transport in Tumor Tissues	601
<i>Mohammad Islam, Sutapa Barua, Dipak Barua</i>	
(582e) Equation-Free Control of Distributed Parameter Systems Using Discrete Empirical Interpolation Method and Proper Orthogonal Decomposition	602
<i>Manda Yang, Antonios Armaou</i>	
(582f) Sampled-Data Event-Triggered Control of Distributed Parameter Systems with Networked Sensors and Actuators	603
<i>Da Xue, Nael H. El-Farra</i>	
(582g) Data-Driven Model Predictive Control of a Seeded Batch Crystallization Process	606
<i>Abhinav Garg, Prashant Mhaskar</i>	
(582h) Model Predictive Control for Linear Distributed Parameter Systems	609
<i>Stevan Dubljevic</i>	
(585a) Autocovariance-Based Plant-Model Mismatch Estimation for Linear MPC with Measurable Disturbances	610
<i>Siyun Wang, Michael Baldea, Leo H. Chiang, Ivan Castillo, Rahul Bindlish, David Stanley</i>	
(585b) Adaptive Multiple-Model Stochastic Predictive Control	611
<i>Tor Aksel N. Heirung, Vinay Bavdekar, Dogan Gidon, Ali Mesbah</i>	
(585c) A Bayesian Filter Switching Strategy for Simultaneous State and Parameter Estimation	612
<i>Aditya Tulsyan, Bhushan Gopaluni</i>	
(585d) Fast Estimation of Plant Steady State, with Application to Static RTO	613
<i>Diogo Rodrigues, Michael Amrhein, Julien Billeter, Dominique Bonvin</i>	
(585e) The Extended and Unscented Kalman Filtering Methods for Real-Time Plasma Insulin Concentration Estimation in an Artificial Pancreas Control System for Patients with Type 1 Diabetes	615
<i>Iman Hajizadeh, Kamuran Turksoy, Eda Cengiz, Ali Cinar</i>	
(585f) Noise Covariance Estimation for an Air Separation Plant	616
<i>Travis Arnold, James B. Rawlings</i>	
(585g) Multi-Rate Moving Horizon Estimation for an Electric Arc Furnace Steelmaking Process	617
<i>Smriti Shyamal, Christopher L. E. Swartz</i>	
(585h) A Simplified Dynamic Model of a Continuous Subsea Oil-Water Gravity Separator for Estimation of Unmeasurable Oil and Water Purities	618
<i>Tamal Das, Johannes Jäschke</i>	
(587a) Schuripopt: A Parallel Optimization Package for Structured Nonlinear-Programming Problems	621
<i>Jose S. Rodriguez, Gabriel Hackebeil, Carl Laird</i>	
(587b) A Scalable Design of Experiments Framework for Infinite-Dimensional Systems	622
<i>Victor M. Zavala, Mihai Anitescu, Jing Yu</i>	
(587c) A Logical Benders Decomposition Algorithm for Binary-Constrained Quadratic Programs with Complementarity Constraints	623
<i>Andreas Waechter, Francisco Jara-Moroni, Frank Curtis, Victor M. Zavala, John Mitchell, Jong-Shi Pang</i>	
(587d) Accelerating the Simplex Algorithm Via Novel Crash Procedures	624
<i>Nikolaos Ploskas, Nikolaos Samaras, Nick Sahinidis</i>	
(587e) Discreetly Discrete: Quietly Adding Integer-Valued Actuators to Model Predictive Control	625
<i>Michael Risbeck, James B. Rawlings</i>	
(587f) Global Optimization of Natural Gas Liquefaction Processes through Differentiable McCormick Relaxations	626
<i>Harry A. J. Watson, Kamil A. Khan, Paul I. Barton</i>	
(587g) Model Predictive Control and Materials Property Estimation of an Industrial Heat Treating Furnace	627
<i>Hari S. Ganesh, Thomas F. Edgar, Michael Baldea</i>	
(597a) A Multidimensional Population Balance Model for Predicting Crystal Size and Aspect Ratio in the Production of Phosphogypsum	628
<i>Zhilong Zhu, You Peng, Kamal Samrane, Allan S. Myerson, Richard D. Braatz</i>	
(597b) Optimal Operation of Batch Enantiomer Crystallization: From Ternary Diagrams to Predictive Control	631
<i>Caio Felipe Curitiba Marcelllos, Helen Durand, Joseph Sangil Kwon, Panagiotis D. Christofides</i>	

(597c) Using Semidefinite Programming to Calculate Bounds on Particle Size Distributions	632
<i>Garrett R. Dowdy, Paul I. Barton</i>	
(597d) Characterization of an Integrated Continuous Cooling Crystallization Process with an in-Situ Wet Mill System for Particle Size Reduction	635
<i>David Acevedo, Vamsi Krishna Kamaraju, Brian Glennon, Zoltan K. Nagy</i>	
(597e) Tailoring the Crystal Size Distribution By Controlling the Crystallization Trajectory in Mass-Count Space	636
<i>Daniel J. Griffin, Martha A. Grover, Yoshiaki Kawajiri, Ronald W. Rousseau</i>	
(597f) Attainable Regions of Particle Sizes for Continuous Milling-Crystallization Processes	637
<i>Thomas Vetter</i>	
(597g) Attainable Regions for Critical Quality Attributes in Drug Manufacture and End Performance	638
<i>Niall Mitchell</i>	
(635a) Surrogate-Based Optimization Methodology for Pharmaceutical Tablet Manufacturing Processes	639
<i>Zilong Wang, M. Sebastian Escotet-Espinoza, Ravendra Singh, Fernando J. Muzzio, Marianthi G. Ierapetritou</i>	
(635b) Probabilistic Robust Optimization and a Posteriori Bounds	640
<i>Yannis A. Guzman, Logan R. Matthews, Christodoulos A. Floudas</i>	
(635c) A Comparative Analysis of Robust Optimization and Scenario-Based Approaches for Optimization Under Uncertainty	643
<i>Logan R. Matthews, Yannis A. Guzman, Christodoulos A. Floudas</i>	
(635d) A Hybrid Data-Driven/Model-Based Framework for the Dynamic Characterization and Refinement of Model Uncertainty in Batch Systems: Application to Robust Online Optimization and Control	644
<i>Francesco Rossi, Gintaras V. Reklaitis, Flavio Manenti, Guido Buzzi-Ferraris</i>	
(635e) Jointly Robust Optimization for Multiple Uncertain Constraints	645
<i>Yuan Yuan, Zukui Li, Biao Huang</i>	
(635f) Multi-Parametric Linear Programming with Global Uncertainty	646
<i>Vassilis M. Charitopoulos, Lazaros G. Papageorgiou, Vivek Dua</i>	
(635g) An Efficient Branch-and-Bound Strategy for Multistage Stochastic Programs with Endogenous and Exogenous Uncertainties	647
<i>Robert M. Apap, Ignacio E. Grossmann</i>	
(635h) Financially Risk-Aware Plant Maintenance Turnaround Planning Incorporating Reliability in Integrated Chemical Sites	648
<i>Sreekanth Rajagopalan, Satyajith Amaran, Nikolaos V. Sahinidis, Scott J. Bury, John M. Wassick</i>	
(636a) On the Systematic Integration of Different Generation Biorefineries	649
<i>Aikaterini D. Mountraki, Ana M. López Contreras, Bouchra Benjelloun Mlayah, Antonis C. Kokossis</i>	
(636b) Use of Multi-Objective Optimization for Selecting Optimally Integrated Biorefinery Processes	650
<i>Ayse Dilan Celebi, Adriano Ensinas, Shivom Sharma, François Maréchal</i>	
(636c) Process Models to Assess the Co-Processing of Gasoil and Bio-Based Feedstocks in Hydroprocessing Unit Operations	651
<i>Asad H. Sahir, Michael Talmadge, Mary Biddy, Mark Bearden, Steven Phillips, Susanne B. Jones</i>	
(636e) Design and Economic Analysis of a Macroalgae-to-Butanol Process Via a Thermochemical Route	652
<i>Chinedu Okoli, Thomas A. Adams, J. Jay Liu, Boris Brigljevic</i>	
(636f) Robust Optimization of Biomass and Natural Gas to Liquid Transportation Fuel Refineries: Process Synthesis Under Uncertainty in Feedstock and Product Prices	654
<i>Logan R. Matthews, Yannis A. Guzman, Onur Onel, Alexander M. Niziolek, Christodoulos A. Floudas</i>	
(636g) Dynamic Modeling of a Continuous Acetone-Butanol-Ethanol (ABE) Fermentation Process	657
<i>Edward Buehler, Ali Mesbah</i>	
(637a) A Multi-Objective Optimization Approach to Optimal Sensor Location Problem in IGCC Power Plant in the Face of Uncertainties	658
<i>Pallabi Sen, Kinnar Sen, Urmila M. Diwekar</i>	
(637b) MILP Formulation for Optimal Planning of Electric Power Infrastructure	659
<i>Cristiana L. Lara, Ignacio Grossmann</i>	
(637c) A Stochastic Optimization Approach for Improving Power Systems Resilience through Operations and Planning	660
<i>Michael Bynum, Bryan Arguello, Brian Joseph Pierre, Andrea Staid, Jean-Paul Watson, Carl Laird</i>	
(637d) An Opportunistic Hybrid Communications System for Distributed PV Coordination and Control	661
<i>S. M. Shafiqul Alam, Tarek Elgindy, Anthony Florita, Bri-Mathias S. Hodge</i>	
(637e) Simulation and Analysis of Power Systems Using Non-Intrusive Appliance Load Monitoring	662
<i>Nikita Patel, Babji Srinivasan, Rajagopalan Srinivasan</i>	
(637f) Effective Variance Reduction and Gradient Estimation Techniques for Stochastic Simulation and Optimization of Microgrids	663
<i>Alphonse Hakizimana, Joseph Scott</i>	
(637g) Operation of Grid Scale Energy Storage Systems: Comparison of Multi-Stage Stochastic Programming and Empe	664
<i>Oluwasanmi Adeodu, Donald J. Chmielewski</i>	
(637h) A Mid-Term, Market-Based Power Systems Planning Model	665
<i>Nikolaos Koltsaklis, Michael C. Georgiadis</i>	
(659a) Identification Methodology for Stirred and Plug-Flow Reactors	666
<i>Alfredo Bermúdez, Noemí Esteban, José L. Ferrín, José F. Rodríguez-Calo</i>	
(659b) A Mixed-Integer Formulation for Online Design of Model Discrimination Experiments	667
<i>Calvin Tsay, Richard Pattison, Michael Baldea</i>	

(659c) Gray-Box Modeling of 300mm Czochralski Single-Crystal Si Production Process	668
<i>Tatsuru Seto, Sanghong Kim, Manabu Kano, Toshiyuki Fujiwara, Masahiko Mizuta, Shinji Hasebe</i>	
(659d) On the Identification of Meta-Models for the Optimization of Grade Transition in Polymerization Processes	675
<i>Zhenyu Wang, Christos Georgakis</i>	
(659e) Error-Triggered on-Line Model Identification for Model-Based Feedback Control	676
<i>Anas Alanqar, Helen Durand, Panagiotis D. Christofides</i>	
(659f) A MINLP Approach to Model-Based Data Mining for the Quick Development of Nonlinear Dynamic Models	677
<i>Marco Quaglio, Fabrizio Bezzo, Asterios Gavriilidis, Enhong Cao, Federico Galvanin</i>	
(659g) Parameter Estimation and Model Discrimination of Batch Solid-Liquid Reactors	680
<i>Yajun Wang, Mukund Patel, Yisu Nie, John Wassick, Lorenz Biegler</i>	
(659h) Development of a Model for a Continuous Ultra-Filtration System	681
<i>Sparsha Jhamb, Rafiqul Gani, Jens-Ulrik Rypke, Carl Wiklund</i>	
(682a) Combined Use of the Sample Average Approximation and the Analytic Hierarchy Process to Support the Design of Chemical Processes Under Uncertainty	682
<i>Dauda Ibrahim, Gonzalo Guillén-Gosálbez, Megan Jobson</i>	
(682b) Using Resilience Principles for Prediction of Loss of Containment Events in Batch Operations	683
<i>Prerna Jain, Efstratios N. Pistikopoulos, Sam Mannan</i>	
(682c) A Demand Response Strategy for Continuous Processes Using Stochastic Optimal Scheduling	684
<i>David Lavoie, Nael H. El-Farra, YueYue Fan, Ahmet Palazoglu</i>	
(682d) Rapid and Accurate Uncertainty Propagation for Nonlinear ODEs Using Nonlinear Solution Invariants	685
<i>Kai Shen, Joseph Scott</i>	
(682e) A Graph Theory Approach to Non-Anticipativity Constraint Generation in Multistage Stochastic Programs with Incomplete Scenario Sets	686
<i>Brianna Christian, Selen Cremaschi</i>	
(682f) Towards Optimal Production of Industrial Gases with Uncertain Energy Prices	688
<i>Natalia Basán, Carlos Méndez, Ignacio Grossmann, Ajit Gopalakrishnan, Irene Lotero</i>	
(682g) MINLP Formulation and Global Solution Approach for Sensor Placement with Non-Uniform Failure Probabilities: Application to Gas Detection Systems	689
<i>Jianfeng Liu, Carl Laird</i>	
(682h) Data-Driven Adaptive Nested Robust Optimization: Modeling Framework and Solution Algorithm for Process Design and Operations Under Uncertainty	690
<i>Chao Ning, Fengqi You</i>	
(684a) Value Based Sensor Network Design	693
<i>Jin Zhang, Donald J. Chmielewski</i>	
(684b) On the Robustness of Economic Nonlinear Model Predictive Control	694
<i>Devin Griffith, Victor M. Zavala, Lorenz Biegler</i>	
(684c) A Carleman Approximation-Based Approach to Address the Performance Criteria Issue of Economic Model Predictive Control Via Lyapunov Method	696
<i>Yizhou Fang, Antonios Armaou</i>	
(684d) Economic Nonlinear Model Predictive Control with a Path-Following Approach	697
<i>Eka Suwartadi, Johannes Jäschke</i>	
(684e) Economic MPC with Local Optimality	698
<i>Su Liu, Jinfeng Liu</i>	
(684f) Multi-Rate Subspace-Based System Identification and Economic Model Predictive Control of the Electric Arc Furnace	699
<i>Mudassir Rashid, Prashant Mhaskar, Christopher L. E. Swartz</i>	
(684g) Tracking Control of Boundary Controlled Continuum Models of Production Systems	700
<i>Xiaodong Xu, Stevan Dujljevic</i>	
(684h) Model Predictive Control for Optimal Zone Tracking	701
<i>Nishith R. Patel, James B. Rawlings</i>	
(703a) A New Multitasking Continuous Time Formulation for Short-Term Scheduling of Operations in Multipurpose Plants	702
<i>Saman Lagzi, Ricardo Fukasawa, Luis A. Ricardez-Sandoval</i>	
(703b) Scheduling Straight Multiproduct Pipelines with Generalized Disjunctive Programming	703
<i>Hossein Mostafaei, Pedro M. Castro</i>	
(703c) Medium-Term Scheduling of Integrated Gasoline Blending and Delivery Operations Using Enhanced Rolling Horizon Decomposition Approach	704
<i>Jie Li, Xin Xiao, Christodoulos A. Floudas</i>	
(703d) Reducing Enterprise Wide Planning and Scheduling to Practice	707
<i>Scott J. Bury, Satyajith Amaran, Bikram Sharda, Eric Foger, Alex Kalos</i>	
(703e) Infeasibility Analysis for Scheduling Applications	708
<i>Apurva P. Samudra, Yash Puranik, Alexander B. Smith, Bijan Sayyar-Rodsari</i>	
(703f) Mathematical Programming Models and Solution Methods for Online Scheduling of Central Heating/Cooling Plants	709
<i>Michael Risbeck, Christos T. Maravelias, Robert Turney</i>	
(703g) A Unified Planning and Scheduling Platform for Refining Operations	710
<i>Dimitrios Varvarezos</i>	
(703h) Continuous-Time Models for Scheduling of Parallel Batch Digesters for Pulp Production	711
<i>Madhup Benawat, Munawar A. Shaik</i>	

(706a) Multivariable Model Predictive Control of a Novel Rapid Pressure Swing Adsorption Process	712
<i>Matthew Urich</i>	
(706b) Model Predictive Control of Atmospheric Pressure Plasma Jets for Biomedical Applications	719
<i>Dogan Gidon, David B. Graves, Ali Mesbah</i>	
(706c) Design and Implementation of Model Predictive Control Strategies for IGCC Power Plant Cycling with Carbon Capture	720
<i>Xin He, Fernando V. Lima</i>	
(706d) Optimal Controller Design Based on Efficient Ant Colony Optimization Algorithm. Case Study: Chemical Process Control	721
<i>Berhane Gebreslassie, Gaurav V. Mirlekar, Fernando V. Lima, Urmila M. Diwekar</i>	
(706e) Stochastic Predictive Control with Closed-Loop Model Adaptation: Application to a Cold Atmospheric Plasma Jet	722
<i>Victoria Ehlinger, Vinay Bavdekar, Dogan Gidon, Ali Mesbah</i>	
(706f) Robust Optimal Dosing Strategy for Bacterial Disinfection	723
<i>Shyam Panjwani, Michael Nikolaou</i>	
(706g) Utilizing Memory in Process Control	724
<i>Jacob Albright, Debangsu Bhattacharyya</i>	
(706h) A Model-Based Framework for Advanced Optimal Operation of Polymerization Processes	725
<i>Navid Ghadipasha, Aryan Geraili, Jose Romagnoli</i>	
(741a) Towards Experimental Validation of a Multi-Resolution Approach for Directed Self-Assembly of Non-Periodic Structures: Spatial Control of Particle Densities	726
<i>Yu Gao, Richard Lakerveld</i>	
(741b) A Hybrid Control Technique to Achieve Spatial and Temporal Control of Droplets in a Microfluidic Device	729
<i>Jeevan Maddala, Raghunathan Rengaswamy</i>	
(741c) Virtual Plant Environment Incorporating Data for Predictive Modeling and Control in Bio-Pharmaceutical Manufacturing	730
<i>Yingying Zheng, Tony Wang, Christian Kunert, Chris Garvin, Cenk Undey</i>	
(741d) Model Predictive Control of Semicontinuous Distillation Process	731
<i>Vida Meidanshahi, Brandon Corbett, Prashant Mhaskar, Thomas A. Adams</i>	
(741e) Regulation of Anemia in Chronic Renal Disease Using Zone Model Predictive Control	732
<i>Jayson McAllister, Zukui Li, Jinfeng Liu</i>	
(741f) A Scale-up Methodology for Continuous Bioreactor Systems Utilizing an Optimal Design Under Optimal Control Constraint Framework	733
<i>Jonathan P. Raftery, M. Nazmul Karim</i>	
(741g) Safety-Based Model Predictive Control with Data-Based Determination of Safety Level Sets	734
<i>Fahad Albalawi, Helen Durand, Anas Alanqar, Panagiotis D. Christofides</i>	
(741h) Advanced Control Automation System of the Syngas Chemical Looping Process: Dynamic Model Simulation and Controller Development	735
<i>Tien-Lin Hsieh, Dikai Xu, Liang-Shih Fan, Andrew Tong</i>	
(760a) Ecosystems As Unit Operations: Designing Integrated Networks of Technological and Ecological Systems	736
<i>Varsha Gopalakrishnan, Bhavik R. Bakshi, Guy Ziv</i>	
(760b) Economic, Environmental and Social Cost Optimization of Biomass Supply Chain for Electricity Generation in WI, USA	737
<i>Sangpil Ko, Jiqing Fan, Pasi Lautala, David R. Shomard</i>	
(760c) Renewable/Fossil Fuel Supply Selection and Supply Chain Optimization for a Synergized Upstream, Downstream and Power Economy System	738
<i>Abdullah Alabdulhadi, Vasilios Manousiouthakis</i>	
(760d) Synthesis of Renewable Energy Supply Networks Considering Different Frequencies of Fluctuations in Supply and Demand	739
<i>Lidija Cucek, Zan Zore, Goran Krajaacic, Mariano Martin, Ignacio Grossmann, Stanislav Boldyryev, Zdravko Kravanja</i>	
(760e) A Holistic Look to Carbon Capture and Use in Sustainable and Economically Enhanced Bio-Based Supply Chains	740
<i>José Miguel Laínez-Aguirre, Mar Pérez-Fortes, Luis Puigjaner</i>	
(760f) Optimal Integration of Renewable Based Processes for Fuels and Power Production: Case Study in Spain	741
<i>Mariano Martin, Ignacio E. Grossmann</i>	
(777a) Designing Functional Materials within the Materials Project	742
<i>Kristin Persson</i>	
(777b) Data Analytics and Machine Learning in Nanomaterials Discovery	743
<i>Michael Fernandez, Amanda S. Barnard</i>	
(777c) Describing the Diverse Geometries of Gold from Nanoclusters to Bulk - A First-Principles Based Hybrid Bond Order Potential	744
<i>Badri Narayanan, Subramanian K.R.S. Sankaranarayanan</i>	
(777d) Topological Data Analysis of Nanoporous Materials Genome Using Pore-Geometry Recognition Technique	745
<i>Yongjin Lee, Berend Smit</i>	
(777e) Unraveling the Role of Pore Topology and Chemical Functionality on the Carbon Capture Performance of Metal-Organic Frameworks	746
<i>Diego Gomez-Gualdron, Edwin Argueta, Randall Q. Snurr</i>	
(777f) An Automated Approach for Developing Graph-Theoretical Cluster Expansions of the Total Energy of Adsorbed Layers	747
<i>Emanuele Vignola, Stephan N. Steinmann, Michail Stamatakis, Phillippe Sauter</i>	

(777g) Property Prediction of Crystalline Solids from Composition and Crystal Structure	748
<i>Bruno A. Calfa, John R. Kitchin</i>	
(777h) Local Pattern Discovery for Uncovering Structure-Property Relationships of Materials	749
<i>Bryan R Goldsmith, Mario Boley, Luca M. Ghiringhelli, Matthias Scheffler</i>	
(777i) Alloy Catalyst Discovery Using Computational Alchemy	750
<i>Karthikeyan Saravanan, O. Anatole von Lilienfeld, John A. Keith</i>	
(777j) To Address Surface Reaction Network Complexity Using Machine Learning, Scaling Relations, and DFT Calculations	751
<i>Zachary Ulissi, Jens K. Nørskov, Thomas Bligaard, Andrew Medford</i>	
(777k) Machine-Learning Acceleration of the Exploration of Potential Energy Surface within Amp	752
<i>Alireza Khorshidi, Andrew A. Peterson</i>	
(778a) Constructing a Framework for Measuring National Energy Security	753
<i>Richard C. Darton, Colin J. Axon</i>	
(778b) Sustainability Analysis of the Supply Chain of Bio-Syngas Production and Its Potential As Chemical Platform for Syngas Fermentation	754
<i>John A. Posada, Baudine Gevers Deynoot, Eduardo Almeida Benalcázar, Henk J. Noorman, Patricia Oxseweijer</i>	
(778c) Design and Operation of Biofuel Supply Chains with Variable Regional Depot and Biorefinery Locations	762
<i>Rex T. L. Ng, John D. Siirola</i>	
(778d) Process Synthesis of Natural Gas to Liquid Transportation Fuels Under Uncertainty: A Robust Optimization Approach	765
<i>Logan R. Matthews, Yannis A. Guzman, Onur Onel, Alexander M. Niziolek, Christodoulos A. Floudas</i>	
(778e) Multi-Scale Operational Planning and Optimal Sizing of Hybrid Renewable Energy System	766
<i>Joohyun Shin, Jay H. Lee, Matthew Realf</i>	
(778f) Modelling the Gradual Expansion of Integrated Wind-Hydrogen-Electricity Networks That Decarbonise the Domestic Transport in Great Britain By 2050	767
<i>Sheila Samsatli, Nouri J. Samsatli</i>	
(778g) A Computer-Aided Scenario Planning of Future Regional and National Energy Systems Based on Feasible Technology Options in Japan	768
<i>Yasunori Kikuchi, Yuichiro Kanematsu, Kazutake Oosawa, Miwa Nakai, Tatsuya Okubo</i>	
Author Index	