Process Development Division

Core Programming Topic at the 2012 AIChE Annual Meeting

Pittsburgh, Pennsylvania, USA
28 October - 2 November 2012

ISBN: 978-1-62276-738-0

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© (2012) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2013)

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

Looking to the Future in Continuous Pharmaceutical Manufacturing 1
Richard D. Braatz

New Challenges and Opportunities for Pharmaceutical Manufacturing Science 2
Vincent Vilker, Mansoor A. Khan

Recent Advances in the Molecular Modeling Foundation of Systems-Based Pharmaceutics 3
Constantinos C. Pantelides

Experience with Regulatory Issues for Biomedical Devices and Vision for the Use of Advanced Control In Pharmaceutical Operations 4
Francis J. Doyle III, Eyal Dassau, Howard Zisser

Chemical Engineering and Biopharmaceutics: Linking the Process with the Ultimate Quality Attribute 5
Ravi M. Shanker

Automating Chemical Kinetics Development and Analysis with the Virtual Kinetics Laboratory 6
Alex Kalos

Electric Power Generation with Sulfur-Based Thermochemical Energy Storage for Concentrated Solar Power 7
Robert T. Buckingham

Effective Global Process Development Team Interactions – From the Lab to the Plant and All Things Between 8
John E. Pace, David B. Hall, Jose Maria Patricio, S. Siva Kumar, Jan Van Den Heijkant

Developing Sustainable Chemical Processes: An Integrated Approach Involving Concurrent Catalyst, Media and/or Reactor Innovations 16
Bala Subramaniam

Polar Functionalization of Polypropylene with Suppressed Molecular Weight Reduction: Near-Ambient Temperature Free Radical Chemistry During Solid-State Shear Pulverization 17
J. Mirian Diop, John M. Torkelson

Novel Molecular Design Techniques for the Design of Systems Involving Chemical Reactions 18
Nishanth G. Chemmangattuvalappil, Vikrant Dev, Mario Richard Eden

Reaction Mechanism Understanding Through Process Development 19
Michelle Mahoney, Frederic Buono, Martin Eastgate, Maxime Soumeillant, Michael Cassidy

Scaled Transport Coefficient Correlations for Fluids 20
Lawrence Novak, Merrill Galloway

Modeling of Foam Flow From Adjacent Pour Regions in Reactive Polyurethane Foaming 28
Christopher J. Hershey, Krishnamurthy Jayaraman

The Role of Open Innovation in Development of Futuristic Technologies for Carbon Capture in Coal-Fired Power Plants: An Academic Perspective 29
Asad H. Sahir, Joann S. Lighty, Lyda Bigelow

Strategies in Advancing the Pharmaceutical Pipeline - An Overview of API Pilot Plant 41
Jim Ratway

A Pharmaceutical Engineering Process/Product Life-Cycle Approach to Drug Product Development and Manufacturing 42
Jose C. Menezes, Stephan Sacher, Georg Scharrer, Stefan Leitgeb, Christine Voura, Simon D. Fraser, Johannes G. Khinast

Leveraging HPLC Data in a QbD Approach, for Right-First Time Scale-up of API Reaction Steps 43
Wilfried Hoffmann, Andrew Bird, Peter Clark

Continuous Distillation Operations and Application of the Wiped Film Evaporator (WFE) to Pharmaceutical Pilot Plant Processing 44
Anne Mohan, Elizabeth Fisher, Rukyah Hennessey, Joe Kukura, Dave Lashen, Crystal Miranda, Glenn Spencer, Michael Ward, Ming Yue, George Zhou

Optimization of Amidecoupling Reaction Conditions Using Kinetic Modeling 47
Ozgur Karahan, Camille O. Anderson, Dimitrios Zarkadas

Scale-up of Superficial Fluidization Air Velocity for a Pharmaceutical Fluid Bed Granulation 48
Brendon G. Ricart, Alan R. Silverman, Kristin J. Ploeger, Edward J. Smith

Experimental Determination of Maximum Shear Stress in Multiphase Flow – From Micro Scale to Pilot Scale Reactors 49
Thomas K. Villiger, Miroslav Soos, Massimo Morbidelli

Effective Application of Established Treatment Technologies for Metals, Metalloids, and Oxyanions 50
James Patterson
Impact of Water Quality and Assessment of Adsorption Technologies for Arsenic Removal 51
Kashinath Banerjee, Gary L. Amy, Tapas K. Das
Removal of Arsenic by a Nano-Particle Blend Hollow Fiber Membrane 53
Jinsong He, J. Paul Chen
Competitive Adsorption of Nickel, Manganese, Chromium and Cadmium From Aqueous Solutions by Different Adsorbents 54
Malyuba A. Abu-Daabes, Hani Abu Qdais, Hatem Alsyouri
Arsenic Mobilization In Alluvial Soils of Punjab, North-West India Under Flooded Conditions 61
Kuldip Singh, Dhanwinder Singh, H. S. Hundal, Raj Kumar
Adsorption of Lead From Aqueous Solutions by Cotton Fabrics Modified with Citric Acid 65
Refugio Bernardo García Reyes, Saúl H. Martínez Treviño, Alcione Garcia González, Ricardo Gómez González
A Model-Based Approach for the Construction of Design Spaces in Quality-by-Design 71
Masako Kishida, Richard D. Braatz
Fluid Bed in a Flash 73
Otto Scheibelhofer, Roland Hohl, Sharareh Salar-Behzadi, Detlev Haack, Kai Koch, Stephan Sacher, Jose C. Menezes, Johannes G. Khinast
From Experimental Data to Building Integrated Dynamic Flowsheet Models for Pharmaceutical Processes 75
Fani Boukouvala, Fernando J. Muzzio, Marianthi Ierapetritou
Modeling and Simulation of a Wurster Column for Particulate Coating Using Population Balance Moldels and Thermodynamics 77
Jianfeng Li, Salvador García-Muñoz, William R. Ketterhagen, James D. Litster
Exceptional Event Managemnt Applied to Continuous Pharmaceutical Manufacturing 79
Anshu Gupta, Gintaras V. Reklaitis, Venkat Venkatasubramanian
Modelling of a Filter Drying Process 80
Giovanni Giorgio, Jason Mustakis, Mark A. Pinto, Sean K. Bermingham
Techno Economic Assessment of a Direct Route to Propylene Oxide 81
Salvador Aldrett, Arian van Mourik, Richard Sebesta
Partial Oxidation of O-Xylene to Phthalic Anhydride Inside of the Explosion Regime Using a Micro Structured Reactor 90
Elias Klemm, T. Lange, S. Heinrich, C. Liebner, H. Hieronymus
Scale-up Approaches to Preserve Particle Properties of Api's in Agitated Filter Driers 94
David Am Ende, Mark T. Maloney
Kilogram-Scale Production of Energetic Materials in a Remote-Controlled Microreactor Plant 95
Stefan Loebbecke
Scale-up of Primary Explosives Using Reaction Engineering Tools 96
Jerry S. Salan
Scale-up of LLM-105 Involving Online Analytics 97
Andrew G. Pearsall
Molecular Design with Simultaneous Topological, Topographical, and Electrostatic Characterization 98
Robert Herring III, Subin Hada, J. Colin Haser, Nishanth G. Chemmangattuvalappil, Mario Richard Eden
Amodeo: Automated Molecular Design Using Optimization 100
Apurva Samudra, Nick Sahinidis
Design of an Emulsified Hand Wash Through a Systematic Model-Based Methodology 101
Michele Mattei, Michael Hill, Georgios Kontogeorgis, Rafiqul Gani
Strategic Search for Experimental Conditions for Efficient Product Design 103
Takuya Kishio, Hiromasa Kaneko, Kimito Funatsu
Data-Driven Optimization of Product Blends Using Multivariate Property Clustering Techniques 105
Subin Hada, Robert Herring III, J. Colin Haser, Nishanth G. Chemmangattuvalappil, Mario Richard Eden
Computer Aided Ionic Liquid Design (CAILD) Method for Development of Green Ionic Liquids 106
Amirhossein Mehrkesh, Arunprakash T. Karunanithi
Layer Melt Crystallization of Long-Chain Aldehydes From Hydroformylation Processes 107
Thorsten Beierling, Gabriele Sadowski
Hybrid Filtration-Drying-Dissolution Device for Compact Pharmaceutical Manufacturing System 108
Shin Yee Wong, Jie Chen, Allan S. Myerson
Design and Characterization of a Continuous Stirred Tank Crystallizer 109
Gary Morris, Guangyang Hou, Mark Barrett, Brian Glennon
X-Ray Compatible Microfluidic Platforms for On-Chip Structure Determination of Membrane Proteins 116
Sudipto Guha, Ashtamurthy Pawate, Sarah L. Perry, Paul J. A. Kenis

Investigation of a Counter-Current Crystallization Process for Separation of Systems Forming Solid Solutions 117
Erik Temmel, Sebastian Wloch, Uwe Müller, Detlef Grawe, Robert Eilers, Heike Lorenz, Andreas Seidel-Morgenstern

Designing a Fit-for-Purpose Agglomeration Method for Pharmaceutical Crystals 119
Chenchi Wang, Daniel Hsieh, Mario Hubert, Chiajen J. Lai

Utilization of Population Balance Models to Develop a Continuous Crystallization Process; Determination of Crystallization Kinetics 120
Christopher L. Burcham, Michael A. Lovette, Christopher S. Polster, Sean K. Bermingham, Hassan Mumtaz

Utilization of Population Balance Models to Develop a Continuous Crystallization Process; Process Design Using Optimization 121
Christopher L. Burcham, Michael A. Lovette, Christopher S. Polster, Sean K. Bermingham, Hassan Mumtaz

Controlling the Composition of a Mixture of Polymorphs by Examining Seeded SMPT Kinetics 122
Ramya Kumar, Venu Nalivela, Srividya Ramakrishnan

Amine-Functionalized Metal-Organic Framework Crystallization Process Design 123
Paul M. Schoenecker, Grace A. Belancik, Bogna Grabicka, William J. Koros, Krista S. Walton

The Role of Meso-Mixing in Anti-Solvent Crystallization Processes 124
Des O'Grady, Mark Barrett, Brian Glennon, Eoin Casey

Crystallization of Active Pharmaceutical Ingredients in Scrapped Surface Crystallizers 125
Jie Chen, Shin Yee Wong, Allan S. Myerson

Continuous Enantioseparation in a MSMPR Crystallizer – Experimental and Theoretical Investigation of Different Process Conditions 126
Kamila Galan, Martin Peter Elsner, Andreas Seidel-Morgenstern

Continuous Crystallization Process Development 127
Haitao Zhang, Justin Quon, James M. B. Evans, Allan S. Myerson, Bernhardt L. Trout

To Teach or Not to Teach, What Is the Answer? 128
Santiago Faucher

Helping Students to Learn by Doing - Capstone Design Experience At Columbia University 129
Michael Hill, Stanley A. Leshaw

Chemical Process Design and Projects Two Semester Sequence 130
Alan W. Weimer

Senior Design At UC Irvine: Process Development and Economics Analysis with PRO/II 131
Gang (Gary) Xu

Conduct Your Capstone Design Class As a Consulting Company 132
Richard L. Zollars

Integrating Active Research On CO_2 Capture in Traditional Process Design 134
Omkar Namjoshi, Paul Nielsen, Matthew Walters, Bo Lu, Siyun Wang, Gary T. Rochelle

Incorporating Process Simulation Across the Chemical Engineering Curriculum to Improve Student Performance On the Capstone Design Project 137
David A. Rockstraw, Martha C. Mitchell

Crystallization Kinetics Identification within a Generic Modeling Framework 138
Kresten Troelstrup Meisler, Noor Asma Fazli Abdul Samad, Nicolas Von Solms, Krist V. Gernaey, Rafiqul Gani

Development of an Empirical Framework for Monitoring CSD Using FBRM in Batch Crystallization 140
Huayu Li, Martha Grover, Yoshiaki Kawajiri, Ronald W. Rousseau

Apply PAT-Enabled Platform to Realize the QbD Control Strategy for Crystallization Processes 141
George Zhou, Aaron Moment, Shane T. Grosser, Paul Fernandez, Luke Schenck, John Higgins

Theoretical and Numerical Analysis of Critical Seed Loading in Batch Crystallization 142
Yu-Ti Tseng, Jeffrey D. Ward

Process Intensification of the Production of Di-Methyl Carbonate (DMC) Using a New Synthesis and Design Process Intensification Methodology 143
Deenesh K. Babi, Johannes Holtbruegge, Philip Lutze, Andrzej Gorak, John Woodley, Rafiqul Gani

A Novel MILP Approach to the Synthesis of Thermally Coupled Distillation Sequences 145
José A. Caballero, Ignacio E. Grossmann

Process Intensification in Ethylene Oxide Production: Optimal Reactor Design From a Process Point of View 151
Hannsjörg Freund, Andreas Peschel, Kai Sundmacher

Microwave Assisted Flow Processing: Coupling of Electromagnetic and Hydrodynamic Phenomena 152
Narendra Patil, Erik Esveld, Faysal Benaskar, Evgeny V. Rebrov, Lumbertus Hulshof, Jan Meuldijk, Volker Hessel, Jaap C. Schouten

Process Intensification for Hydrogen Generation Using Micro-Channel Steam Reforming 156
Peter Bossard, Jacob Mettes, Luis Breziner, Benjamin A. Wilhite

Kinetic Modeling of Methanol to Olefins (MTO) On SAPO-34 Catalyst 164
Guozhen Qi, Siqing Zhong, Hongyuan Zong
Numerical Investigation of Effect of Hollow Cross-Over Disk On Flow and Heat Transfer in Tube of Cracking Furnace 165
Yuan Zong, Xiaogang Yang, Ling Zhao
Evaluation of Process Capability and Robustness for a Lyophilized Product 166
Michael M. Choi, Daniel Kim, Marazban Sarkari, Ronald Simko, David Unger, Stelios Tsinontides
Understanding Thermodynamics of Aqueous Film Coating Process Using Data Logger 167
Ganeshkumar A. Subramanian, P. Pandey, S. Gour, D. Bindra, S. Badawy
Process Robustness Aided by Retrospective Multivariate Data Analysis of Factory Data - A Case Study 168
Sankar Raghavan, Jeffrey Foster, Dale Kopas, Ed Warner
Application of Weber Number-Based Regime Map for Scaling and Control of Pharmaceutical Coating Sprays 170
Sip C. Liew, Ariel Muliadi, Paul Sojka
Characterizing Heterogeneity of Environmental Conditions in Various Bioreactor Scales Used for Cell Cultivation 171
Miroslav Soos, Benjamin Neunstoecklin, Massimo Morbidelli
Microchannel Rapid Temperature Swing Adsorption of CO_2 for Methane Production 172
Kriston Brooks, Scot Rassat, Paul Humble
Solubilities of CO_2 in Aqueous Solutions of Ionic Liquid and Monoethanolamine 173
Fan Xu, Haifeng Dong, Xiangping Zhang, Hongshuai Gao, Zhanli Wang, Suojiang Zhang, Baozeng Ren
A Nove Amino-Functionalized Ionic Liquid for CO_2 Capture 174
Jinzhi Zhang, Haifeng Dong, Xiangping Zhang
Assessing Anhydrous Tertiary Alkanolamines for Gas Purifications 175
David J. Heldebrant, Paul M. Mathias, Kash Afshar, Satish Reddy, Arnold R. Smith, Rubin J. McDougal, Louis V. Jasperson, Phillip K. Koech, Mark Bearden, Charles J. Freeman
Development of a Novel Carbonate Absorption Process with Crystallization-Enabled High Pressure Stripping for Post-Combustion CO_2 Capture: Kinetic Study of Bicarbonate Salt Crystallization 176
Qing Ye, Manoranjan Sahu, Yongqi Lu, Xinlei Wang
Doped Lithium Orthosilicate for Absorption of CO_2 At Steam Atmosphere with Low CO_2 Partial Pressure 177
Qi Zhang, Yang Liu, Qian Ye, Dongmei Sun, Zibin Zhu
Data Integration in Pilot Plants for Goal Optimization 185
Hsiang Yee Lai
Pilot-Scale Testing of an in Tank Process to Remove Radionuclides From Waste Water 186
Michael Poirier
Benchmarking of a New Absorption Mini-Plant 187
Chinmay Kale, Philip Lutze, Andrzej Górak
Development of a Short-Cut Model for Three-Phase Liquid Separation Dynamics for a Hydroformylation Mini-Plant 188
David Müller, Erik Esche, Michael Müller, Günter Wozny
Detection and Diagnosis of Blockage in Externally Parallelized Microreactors 190
Osamu Tonomura, Shinji Hasebe
Integration of Pervaporation in the Methyl Acetate Synthesis 191
Thomas Winkler, Susanne Lux, Matthäus Siebenhofer
From Racemate to Single Enantiomer with 100% YIELD 192
Markus Fuereder, Christian Femmer, Sven Panke, Matthias Bechtold
Reactive Distillation for Synthesis of Ethyl Levulinate From Biobased Resources 193
Aspi K. Kolah, Lars Peereboom, Kelly O'Connell, Carl T. Lira, Dennis J. Miller
Experimental Investigation and Model Validation of a Heterogeneously Catalyzed Reactive Distillation Process to Intensify the Synthesis of n-Butyl Acrylate From Acrylic Acid and n-Butanol 194
Alexander Niesbach, Ron Fuhrmeister, Jan Daniels, Benjamin Schröter, Philip Lutze, Andrzej Górak
Off-Cut Recycling in Batch Reactive Distillation Processes 197
Yu-Lung Kao, Jeffrey D. Ward
Optimal Design of Catalytic Distillation Column for the Hydrolysis of Methyl Acetate 198
Huidong Zheng, Yanru Zeng, Suying Zhao, Jiaojiao Bai
Process Improvements Through Heat Integration in Distillation Schemes: Design and Retrofit 211
Faisal Baksh
Concentrate Enhanced Recovery Reverse Osmosis: A New Process for RO Concentrate and Brackish Water Treatment 212
Anthony Tarquin, Guillermo Delgado

Demonstration of Zero Discharge Desalination Technology for Concentrate Management 220
Tom Davis, Brad Biagini, Malynda A. Cappelle, Bernie Mack, Lawrence Jessup, Holly Johnson, Emily Gilbert
Water Purification with Closed Circuit Reverse Osmosis 223
Richard Stover
A Detail Analysis of the Performance of Different Antiscalants in Calcium Sulfate Supersaturated Brackish Water 225
Anthony Tarquin, Guillermo Delgado
Purity of NaCl in the Electrodialysis Metathesis (EDM) Process for Water Desalination 227
Lucy Mar Camacho, Tom Davis, Malynda A. Cappelle
Assessing the Potential for Large-Scale Utilization of Fossil-Fuel Derived CO_2 228
Jared Ciferno, John J. Marano
Some Perspectives On the Use of Solar and Other Renewable Energy to Facilitate Carbon Management 229
Robert Wegeng
Carbon Capture and Storage Directly From Flue Gas: The Effects of Chemical and Biological Catalysts On Magnesium Carbonate Formation 230
Edward J. Swanson, Patrick V. Brady, Ah-Hyung Alissa Park
Environmentally Benign Processes for Absorption and Chemical Fixation of CO_2 231
An-Hua Liu, Ran Ma, Liang-Nian He Sr.
Process Ecoefficiency of Methanol and Dmc Production From CO_2: A Comparative Analysis 232
Camila Ribeiro, José L. Medeiros, Ofélia Araújo, Paulo Coutinho, Rita M. B. Alves
High Efficiency Direct Electrochemical Conversion of CO_2 to Liquid Fuel 233
Jingjie Wu, Frank Risalvato, Fusheng Ke, Perry Pellechia, Xiao-Dong Zhou
Electrochemical Conversion of Carbon Dioxide to Useful Products 234
Arun Agarwal, Shan Guan, Davion Hill, Edward Rode, Narasi Sridhar
Process Intensification by Membrane-Assisted Reactive Separation Processes: A Design Tool Based On Process Analysis and Optimization 235
Johannes Holtbruegge, Deenesh K. Babi, Philip Lutze, Raifqul Gani, Andrzej Górak
New Vapor Compression Alternatives in Thermally Coupled Distillation 237
José Antonio Caballero, Miguel A. Navarro, Juan A. Reyes-Labarta
Development of New Designs of Oscillatory Mesoscale Baffled Reactor for Continuous Biodiesel Production 243
Anh N. Phan, Adam P. Harvey
Nano-TiO_2 Sol-Gel Synthesis in the Spinning Disc Reactor 252
Somaieh Mohammadi, Kamelia Boodhoo
Shared Research for Process Intensification – An Example Project 258
Leon Geers, Axel Lexmond, Murk van Rooijen
Effect of Sulfur Poisoning On A Cobalt-Based Fischer-Tropsche Catalyst in A Fixed BED Compact HEAT Exchange Reactor 259
Hani Gadalla, Steven J. Vallee, Zhijun Jia, Burtron H. Davis, Dennis E. Sparks
Thermophiles for Biofuels Production 260
Lew P. Christopher
Using a Recombined Microorganism Consortium for One-Step Production of Ethanol and Hydrogen Directly From Cellulose 261
Ran Du, Shizhong Li
Low Cost and Low Energy Consumption Process to Convert Soluble Sugar and Homocelluloses in Sweet Sorghum Stalks Into Ethanol 262
Jihong Li, Bing Han, Shi-Zhong Li
Xylose Fermentation and Respiratory-Deficiency in Saccharomyces Cerevisiae 263
Adel Ghaderi, Benjamin L. Wang, Hang Zhou, Gregory N. Stephanopoulos
Evaluation of a Pilot-Scale Facility for Biocrude Production by Activated Sludge Cultures Via Lignocelullose Sugar Fermentation and Downstream Recovery Processes 264
Andro Mondala, Rafael Hernandez, Todd French, William Holmes, Magan Green, Linda McFarland, Larry Pearson, Jesse Simmons, Robert Glenn, Brady Biggers
Optimization of Extracellular Polymeric Substance (EPS) Production by Activated Sludge Via Fermentation of Glucose 265
Hien Nguyen, Patrisha Pham, Rafael Hernandez, Todd French, Andro Mondala
Enzymatic Hydrolysis of Cellulosic Biomass in Nonaqueous Solvents 266
Vance Jaeger, Jim Pfaendtner

Application of Quality by Design Principles for An Existing Product for the Control of the Dimer Impurity in the Manufacturing Process 267
Gautam Samanta, Praveen K. Sharma, S. Srividhya, Kamlesh Pai Fondekar, K. R. Janardan Sarma, Saurabh Gupta, G. R. B. Ravish, Y. Raghuram

Investigation of the Impact of Mode of Operation (Batch vs Flow) On Design Space Map 274
Shankar Vaidyaraman, Sze Wing Wong, Shekhar K. Viswanath

A QbD Approach to the Process Development of Tofacitinib 275
Bob Dugger

Design of a Pharmaceutical Manufacturing Process Using QbD Principles: The Challenge of Technical Transfer to Manufacturing and Lifecycle Development 276
Conor Collins, Steve Ball

Strategy and Process for Effective Scale-up On the Removal of Pd During the Synthesis of A Drug Substance 277
Alexander Chu-Kung, Hsien-Hsin Tung

Implementation of Reaction Modeling and Process Analytical Technology in Design Space Development 278
Daniel Hallow, Michael Fenster, Antonio Ramirez, Robert Wethman, Nathan Domagalski

Application of Quality by Design in API Process Development 279
Nirav Shah, Erik Johansson

Utilizing Thermochemical Process Streams to Upgrade Bio-Char Into Value Added Activated Carbon Through Physical Activation 280
Joseph Polin, Zhengrong Gu

Optimum Parameter Selection and Modeling of Batch Extraction of Betulinic Acid From Leaves of Vitex Negundo Linn 282
Suyog V. Taralkar, Sujay Chattopadhyay, Vilash G. Gaikar, Pinjala V. Vijaybabu, A. K. Ray

Conversion of Carbohydrates to Chemicals in Hot Water Using SO_2 As a Recoverable Catalyst 296
Yucui Hou, Weina Liu, Shidong Tian, Weize Wu

Extraction of Value-Added Chemicals From Fast Pyrolysis Oils 300
Duo Wang, Dong-Can Lv, Yun-Quan Liu

Biochar Based Activated Carbon As Adsorbent to Recover Volatile Chemicals From Photobioreactor 306
Zhengrong Gu, Joseph Polin, Xiaomin Wang, Muthu Ramanathan, Kasiviswanathan Muthukumarappan

Prediction of Weak Acid Toxicity in S. Cerevisiae Using Genome-Scale Models 307
Patrick B. Hyland, Serene Lock Sow Mun, Radhakrishnan Mahadevan

Optimal Design of LNG Plant for Cost Minimization 309
Jeongwoo Jeon, Kiwook Song, Jeongnam Kim, Chonghun Han

Mitigation of Refinery Pre Heat Train Fouling by Optimisation of Operating Conditions and Application of Heat Exchanger Technologies 310
Marion Ratel, Zoé Minvielle-Anxionnaz, Yash-Vardhan Kapoor, Luc Seminel, Bernard Vinet

Enhanced Development and Control of Continuous Processes Using Real Time in Situ FTIR Analytics 318
Sean Cusack

Analysis of the Influence of Heat Flows in Optimal Design and Operation of Multicomponent Distillation Columns: Extractive Distillation Case Study 319
Arley F. Nova, Manuel A. Ramos, Jorge Mario Gómez

A Hybrid Simulation-Optimization Approach for the Design of Internally Heat-Integrated Distillation Columns 321
Juan A. Reyes-Labarta, Miguel A. Navarro, José Antonio Caballero

Design of Reactive Distillation Process for the Production of n-Butyl Levulinate 328
Tzu-Hsuan Peng, Cheng-Liang Chen, I-Lung Chien

Application of Plasma Electrolysis Technology in Chlor Alkali Production Sector 329
Fakhrian Abqari

Teaching Product with Process Design 330
Warren D. Seider

The Teaching of Capstone Design 331
David L. Silverstein, Lisa G. Bullard, Warren D. Seider, Margot A.-S. Vigeant

Drug Product Model Design, Development, Qualification, and Maintenance in a QbD Framework 332
Hayden Thomas

Prediction of Post-Relaxation Radial Tensile Strength of Pharmaceutical Tablets Using At-Line Collected near Infrared Data 333
Sameer Talwar, Benoit Igne, Zhenqi Shi, Carl A. Anderson, James K. Drennen III

Quantitative Analysis of Crystalline Materials in Binary Compacts Using Time Domain Spectra of THz Spectroscopy and Density Dependence 334
Md. Anik Alam, James K. Drennen III, Carl A. Anderson

Bulk and Micro-Scale Characterization of Continuous Powder Blending Integrated with an Multi-Point in-Line NIR As a PAT Tool 335
Juan G. Osorio, William E. Engisch Jr., Fernando J. Muzzio

Effect of Lubricant Mixing Time and Concentration, Compaction Speed and Compression Force On the Dissolution Profile of a Control Release Formulation 336
Sarang Oka, Pallavi Pawar, Fani Boukouvala, Fernando J. Muzzio

QbD Case Studies: An Integrated Multivariate Approach to Drug Product and Process Development 338
Goldi Kaul

Automation and Control of Drug-On-Demand Technology 343
Laura Hirshfield, Arun Giridhar, Gintaras V. Reklaitis, Michael T. Harris, Venkat Venkatasubramanian

Exergy-Loss-Minimization Based Process Synthesis for Cascade Refrigerant System in Ethylene Plants 344
Ha Dinh, Jian Zhang, Qiang Xu

Development of the Optimal Flowsheet of Isomerization of Light Gasoline Fractions 345
Nickolay V. Kuzichkin

A Systematic Framework for Synthesis and Design of Multi-Scale Processing Networks Using Incremental-Based Solution Strategy 346
Alberto Quaglia, Maxim Shishmarev, Bent Sarup, Gürkan Sin, Rafiqul Gani

Design of a Reactive Distillation Column: Comparison Between Trays and Packings 348
Paola Bastidas, Julio C. Vargas, Alvaro Orjuela, Iván D. Gil, Gerardo Rodriguez

A State-Space-Based Mixed Integer Dynamic Optimization Formulation for Batch Distillation Process Synthesis 349
Shan Jin, Hong-Guang Dong, Xinwen Guo

Design and Synthesis of Energy Integrated Multipurpose Batch Plants Using a Robust Scheduling Platform 358
Esmael Reshid Seid, Thokozani Majozi

Global Optimization of Nonconvex MINLP Problems by Domain and Image Partitioning with Applications to Heat Exchanger Networks 359
Sung Young Kim, Debora Faria, Miguel Bagajewicz

An Integrated Methodology for Design of Tailor-Made Blended Products: Biofuels and Bio-Based Lubricants 360
Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley, Rafiqul Gani

Process Synthesis and Technoeconomic Evaluation of a Catalytic Biomass-to-Fuels Strategy 361
Sercan Murat Sen, David Martin Alonso, Stephanie G. Wettstein, Elif I. Gurbuz, Carlos A. Henao, James A. Dumesic, Christos T. Maravelias

Use of Octanol-Water Partition Coefficient and Toxicity Prediction in Design of Ionic Liquids for in Situ Fermentation Extraction 362
John White, Brock C. Roughton, Kyle V. Camarda, Aaron M. Scurto

Bio-Based Gasoline Additives: Product and Chemistry Selection Through Network Generation and Optimization 363
W. Alex Marvin, Srinivas Rangarajan, Prodromos Daoutidis

On the Systematic Synthesis Screening and Integration of Real-Life Biorefineries 364
Marinella Tsakalova, Athanassios Nikolakopoulos, Antonis Kokossis

Integrated Pathway Optimization for Biorefineries 365
Pascual Eduardo Murillo-Alvarado, Ismael Leonardo Razo, Medardo Serna-González, Mahmoud El-Halwagi

Optimization of Biochemical Conversion Process of Lignocellulosic Biomass to Sugars by Integrating the Kinetic Models 372
Vasanth Natarajan, Iftekar A. Karimi

Simplified Life Cycle Analysis As a Route to Fast Decision Making in Product and Process Development for Sustainability 373
Santiago Faucher

Process Development for a Higher Quality and Cost Optimized Monomer 374
Ahmed A. Youssef, Mohan Khadilkar

Carbon Footprint Analysis of Dairy Feed From a Mill in Michigan, USA 375
Felix Adom, Greg Thoma, David R. Shonnard

Urban Mining: A Process and Technology Review 376
Daniel Brosig

Sizing of a Packed Reactive Distillation Column for Isoamyl Butyrate Production Using an Equilibrium Model 377
Jairo A. Duran, Karen A. Cañon-Rubio, Alejandro Lopez Gomez, Alvaro Orjuela, Gerardo Rodriguez

Analysis of Alternative Processes for Anhydrous Ethanol Production, an Economic and Environmental Approach 378
Michel Kahwaji Janho, Jorge E. Gatica, María Rosa Hernández, Fernando Daniel Mele, Mauricio Colombo
Examining Correlations of Electrostatic Discharge Sensitivity and Electrical Conductivity of Composite Energetic Materials 380
Eric Collins, Chelsea Weir, Michelle Pantoya
Nanoscale Aluminum, Silicon, and Aluminum/Silicon Mixture Formation for Use in Pyrotechnic Applications 381
Mark Miller, Zac Doorenbos, Matt Puszynski, Lauren Armstrong, Deepak Kapoor, Jan Puszynski
On Mechanism of Thermal Initiation in Fully-Dense 2Al.3CuO Nanocomposite Powder 388
Rayon Williams, Mirko Schoenitz, Alexandre Ermoline, Edward L. Dreizin
Particle Design of HMX Using Supercritical Anti-Solvent Processes 389
Bumjoon Seo, Youn-Woo Lee, Byung-Chul Lee, Hyoun-Soo Kim
Nanostructured Aluminum-Fluorocarbon Particles for Energetic Applications 390
Travis R. Sippel, Steven F. Son, Lori J. Groven
Combustion of Nanoscale Silicon with Polytetrafluoroethylene 391
Brandon C. Terry, Lori J. Groven, Paul Redner, Youdong Lin, Alexander Mukasyan, Deepak Kapoor, Steven F. Son
Optimal Design of Integrated Electric-Power and Algal Biofuel Generation Systems 392
Cesar Giovani Guitierrez-Arriaga, Medardo Serna-González, José María Ponce-Ortega, Mahmoud El-Halwagi
Degradation of of Rhodamine B Dye Over Mn-Doped Titania Nanotubes 399
Manohar Palla, Rakesh Sadu, R. Asapu, George W. Spencer, Jewel Andrew Gomes, Zhanhu Guo, Daniel H. Chen
Bio-Inspired Green Approach to Manufacture Fibers 400
Kadhiravan Shanmuganathan, Robert K. Sankhagowit, Prashanth Iyer, Christopher J. Ellison
Reducing Water Usage in Bioprocessing 401
Demetri Petrides, Charles Siletti
Green Approach to Produce Bio-Jet Fuel From Microalgae 402
Marian Elmoraghy, Ihab Farag
Impact of Floc Size On Ethanol Tolerance of the Self-Flocculating Yeast SPSC01 and Underlying Mechanism 404
Chuang Xue, Feng-Wu Bai
Substantial Involvement by DOE to Address Scale-up Challenges for Biorefineries 405
Gene R. Petersen, Glenn Doyle, Art Wiselogel, Carol Babb, Andras Marton
Scale up of IH^2 Process for Converting Biomass to Gasoline and Diesel 410
Terry Marker, Martin Linck, Michael Roberts, Pedro Ortiz-Toral, Jim Wangerow, Larry Felix
Piloting a Multiproduct Biorefinery 411
James J. Foster, Michael Erpelding
Scale-up of Ethanol Production From Sweet Sorghum Stems Using Advanced Solid-State Fermentation Technology 412
Shi-Zhong Li, Lei Zhang
Evaluation of Bio-Oil Corrosion Characteristics 413
Patrick Johnston, Robert C. Brown
Author Index