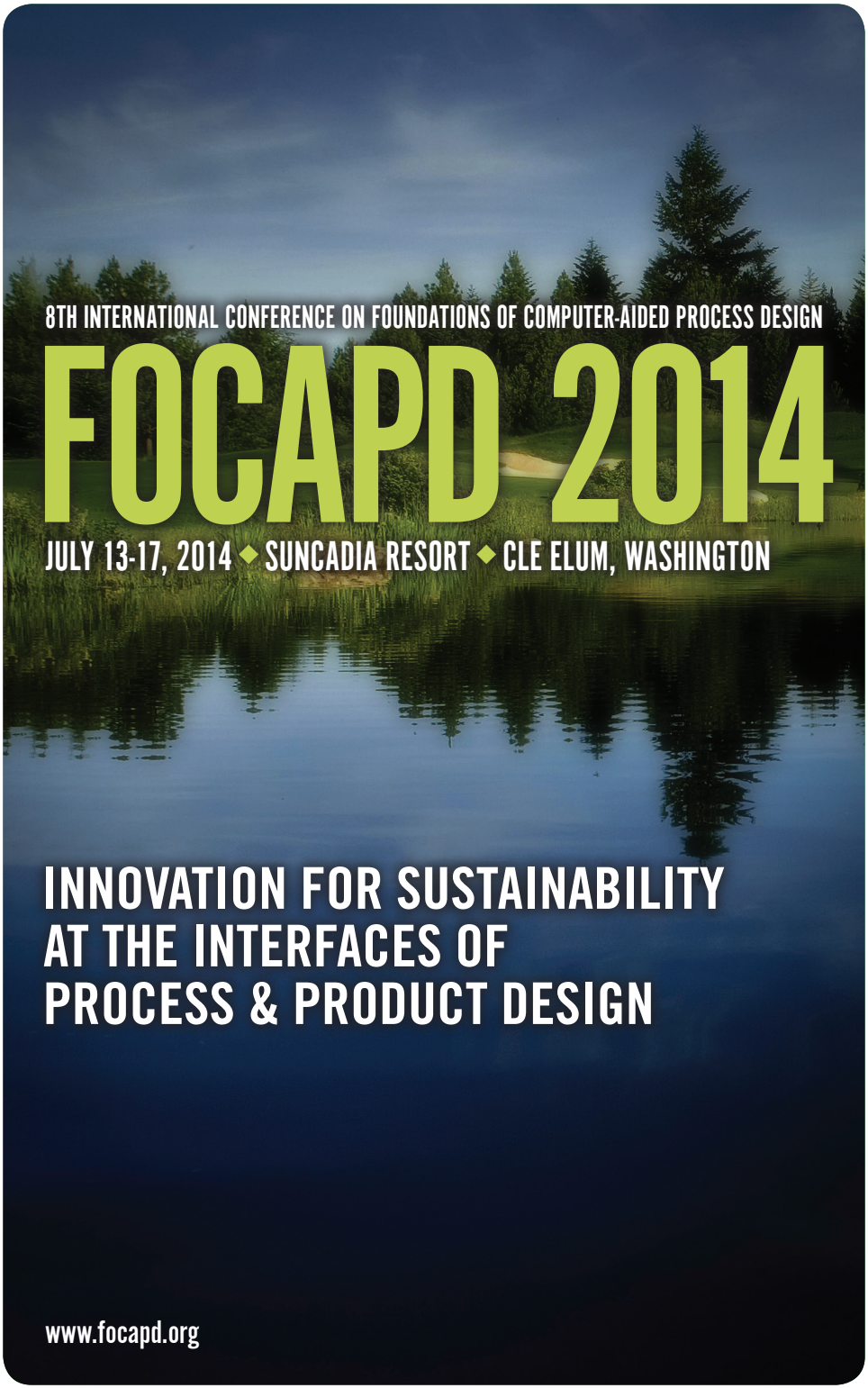
8TH INTERNATIONAL CONFERENCE ON FOUNDATIONS OF COMPUTER-AIDED PROCESS DESIGN
FOCAPD 2014
JULY 13-17, 2014 ◆ SUNCADIA RESORT ◆ CLE ELUM, WASHINGTON
INNOVATION FOR SUSTAINABILITY
AT THE INTERFACES OF
PROCESS & PRODUCT DESIGN
www.focapd.org

FOUNDATIONS OF COMPUTER-AIDED PROCESS DESIGN (FOCAPD 2014)

Innovation for Sustainability at the Interfaces of Process and Product Design

JULY 13-17, 2014 ◆ SUNCADIA RESORT ◆ CLE ELUM, WASHINGTON ◆ WWW.FOCAPD.ORG

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Auburn University

JOHN D. SIIROLA
Sandia National Laboratories

GAVIN P. TOWLER
Honeywell/UOP

CONFERENCE MANAGER

ROBIN CRAVEN
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SCOPE OF FOCAPD 2014

The Foundations of Computer-Aided Process Design (FOCAPD) is the premier international conference focusing exclusively on the fundamentals and applications of computer-aided design for the process industries. Held every five years, FOCAPD 2014 is the eighth in this series, and brings together researchers, educators and practitioners to identify new challenges and opportunities for process and product design. The chemical industry is entering a new phase of rapid evolution. The availability of low-cost feedstocks from natural gas is causing renewed investment in basic chemicals, while societal pressures for sustainability and energy security continue to be key drivers in technology development and product selection. This dynamic environment creates opportunities to launch new products and processes and to demonstrate new methodologies for innovation, synthesis and design. FOCAPD 2014 will foster constructive interaction among thought leaders from academia, industry, and government and provide a showcase for the latest research in product/process design.

SUNCADIA RESORT

FOCAPD 2014 will be located at the Suncadia Resort on the sunny eastern slopes of the Cascades, 85 miles from Seattle, Washington. The resort offers outdoor recreation, luxurious accommodations and amenities, and state-of-the-art facilities.

Call their toll-free number: 866-904-6300 or 425-373-3598. Please ask for the FOCAPD room block.

Deluxe Guestroom	$169.00 + resort fee + tax
One Bedroom Suite	$219.00 + resort fee + tax
Two Bedroom Suite	$388.00 + resort fee + tax

These rates are available from July 10 to July 20.

www.suncadiaresort.com

TECHNICAL AREAS

In the context of the theme of the conference "Innovation for Sustainability at the Interfaces of Process and Product Design" we solicited papers that emphasize the impact of computer-aided design on sustainability both within traditional chemical processes and at the interface of traditional processes with non-traditional areas. We encouraged papers from all areas of systems, process, and product design, with particular emphasis on the following areas:

- Design for sustainability and energy efficiency
- Process design and the future smart grid
- Impact and opportunities arising from abundant shale gas
- Design for carbon capture and sequestration
- Design of non-traditional energy systems
- Design of sustainable supply chains
- Advances in process intensification
- Integration of risk modeling, uncertainty quantification, and process design
- Future process and product design education
- Bio- and pharmaceutical process design
- Design for safety
- Integration of dynamics, controllability, and process design
- Emerging tools for product and process design

A highlight of the FOCAPD series has been the interactive contributed paper sessions. In this tradition, all contributed papers will be presented as posters at the conference. Guidelines for preparation and submission of contributed papers are available at **www.focapd.org**

CONFERENCE PROCEEDINGS

All accepted contributed and invited papers will be included in the conference proceedings as part of the Elsevier book series Computer Aided Chemical Engineering. This provides a fully archival and indexed record of the conference and aligns the FOCAPD meeting with the other major design conferences such as the ESCAPE and PSE series, which both publish their proceedings as part of this book series. In addition, selected full length papers from the conference will be published in a special issue of Computers and Chemical Engineering.

REGISTRATION

The conference fee includes one copy of the proceedings book (electronic format), the opening reception, refreshments at the poster sessions, evening hospitality, and the conference banquet.

Early registration (prior to May 1, 2014)	$995
Standard registration	$1195
Student registration	$495

TRAVEL SUPPORT FOR JUNIOR RESEARCHERS

The conference organizers have secured travel support for graduate students, postdoctoral researchers, and junior faculty through both federal and industrial sponsorships. A detailed description of the application procedure is available on the conference website.

INVITED SPEAKERS

THOMAS ADAMS II
McMaster University
Challenges and Opportunities in the Design of New Energy Conversion Systems

CLAIRE ADJIMAN
Imperial College London
Molecules Matter: The Expanding Envelope of Process Design

MICHAEL BALDEA
University of Texas at Austin
Multum in Parvo:
A Process Intensification Retrospective and Outlook

PAUL BARTON
MIT
Design of Microbial Consortia for Industrial Biotechnology

LORENZ BIEGLER
Carnegie Mellon University
MPCCs and ROMS: New Paradigms for Multi-scale Process Optimization

SCOTT BROWN
Invensys
Some Thoughts on the Next Generation of Process Simulators

KYLE CAMARDA
University of Kansas
The Future of Chemical Engineering Design:
Impact of Faculty Makeup and Industrial Needs

NISHANTH CHEMMANGATTUVALAPPIL

University of Nottingham – Malaysia

Challenges and Opportunities in Computer Aided Molecular Design

SELEN CREMASCHI

University of Tulsa

A Perspective on Process Synthesis: Challenges and Prospects

MICHAEL DOHERTY

University of California — Santa Barbara

Product and Process Design for Particulate Solids: Recent Progress and Future Challenges

CHRISTODOULOS FLOUDAS

Princeton University

A Novel Framework for Carbon Capture, Utilization, and Sequestration, CCUS

RAFIQUL GANI

Technical University of Denmark

Product Design – From Molecules to Formulations to Devices

IGNACIO GROSSMANN

Carnegie Mellon University

Optimization Models for Optimal Investment, Drilling and Water Management in Shale Gas Supply Chains

DIANE HILDEBRANDT

University of South Africa

Addressing a Design Defect: Process Targets and Flowsheets

MICHAEL HILL

Columbia University

The Future of Chemical Engineering Design: impact of Faculty Makeup and Industrial Needs

JAKOB HUUSOM

Technical University of Denmark

Integration of Design and Control

MARIANTHI IERAPETRITOU

Rutgers University

Challenges and Opportunities in Pharmaceutical Manufacturing Modeling and Optimization

M. NAZMUL KARIM

Texas A&M University

Viable Alternatives for Biofuels using Biochemical Pathways

IFTEKHAR KARIMI

National University of Singapore

Perspectives on the Design and Planning of Oil Field Infrastructure

ANTONIS KOKOSSIS

National Technical University of Athens

Design of Integrated Biorefineries

CARL LAIRD

Purdue University

Design Software: Challenges and Opportunities

AJAY LAKSHMANAN

Aspen Technology

Transformation of Process Engineering — A Software Perspective

PATRICK LINKE

Texas A&M University – Qatar

On the Development of Strategies for Water and Energy Management in the Context of the Water-Energy-Food Nexus

M. SAM MANNAN

Texas A&M University

Process Safety at the Crossroads of Systems Engineering, Complex Systems, and Engineering for Sustainable Development

CHRISTOS MARAVELIAS

University of Wisconsin

Process Systems Engineering for Renewable Energy: Lessons Learned, Challenges, and Opportunities

CARL MESTERS

Shell

Making More Molecules for Mobility & Materials

DAVID MILLER

National Energy Technology Laboratory

Advanced Computational Tools for Optimization and Uncertainty Quantification of Carbon Capture Processes

KA NG

Hong Kong University of Science and Technology

Product Design – From Molecules to Formulations to Devices

PATRICK PICCIONE

Syngenta

Industrial Reflections on Modelling of Fine Chemicals and Seeds Process/Product Design

EFSTRATIOS PISTIKOPOULOS

Imperial College London

A Framework for the Design, Modeling and Optimization of Biomedical Systems

GINTARAS REKLAITIS

Purdue University

Perspectives on Systems Engineering Advances in Process and Product Design

JEFFREY SEAY

University of Kentucky – Paducah

Developing a Taxonomy for the Key Principles of Design and Education for Sustainability

WALT WOLTOSZ

Simulations Plus

Recent Advances In Computational Tools for Pharmaceutical Research and Development

FENGQI YOU

Northwestern University

Integration of Supply Chain Design and Operation: Challenges and Opportunities

TECHNICAL PROGRAM OVERVIEW

	SUNDAY July 13	MONDAY July 14	TUESDAY July 15	WEDNESDAY July 16	THURSDAY July 17
Morning	–	Plenary Lectures	Plenary Lectures	Plenary Lectures	Plenary Lectures
Afternoon	Registration	Plenary Lectures	Plenary Lectures	Plenary Lectures	Plenary Lectures
Evening	Welcome Reception Opening Lecture	Poster Session 1 Hospitality	Poster Session 2 Hospitality	Poster Session 3 Hospitality	Banquet Closing Lecture

CONTRIBUTED PAPERS

The contributed papers sessions will be a significant highlight of FOCAPD 2014 and will focus on poster presentations of recent results, methods, and applications in Computer-Aided Product and Process Design. The response to the call for contributed papers has been very strong, and 96 papers have been accepted for presentation in the contributed papers sessions (up almost 30% from FOCAPD 2009). To accommodate the papers and to ensure excellent interaction among all conference attendees, the contributed papers will be divided into three separate and non-overlapping poster sessions scheduled for Monday, Tuesday, and Wednesday evenings.

Spatially Constrained Interplant Water Network Synthesis with Water Treatment Options
Sabla Alnouri, Patrick Linke, and Mahmoud M. El-Halwagi

Revisiting the Simultaneous Process Optimization with Heat Integration Problem
Rahul Anantharaman, Erik Lien Johnsen, and Truls Gundersen

A Framework for the Modelling of Biphasic Reacting Systems
Amata Anantpinijwatna, Gürkan Sin, John P. O'Connell, and Rafiqul Gani

Sustainable Process Synthesis-Intensification
Deenesh K. Babi, Johannes Holtbruegge, Philip Lutze, Andrzej Górak, John M. Woodley, and Rafiqul Gani

Towards Multi-period Planning of Direct Reuse Water Networks in Industrial Cities
Sumit Bishnu, Patrick Linke, and Mahmoud El-Halwagi

Superstructure Optimization: Reaction Yield Dependent CO2 Removal from OCM Product Gas
Christian Bock, Erik Esche, David Müller, and Günter Wozny

Air Quality Considered Site Selection for New Chemical Plants
Tianxing Cai, Sujing Wang, and Qiang Xu

Sustainability Assessment Methodology for Process and Product Design of Appropriate Technology for Developing Regions
William R. Croft and Jeffrey R. Seay

Characterization Based Reverse Design of Ionic Liquids
Sarah E. Davis, Subin Hada, Robert H. Herring III, and Mario R. Eden

Reactant Structure Generation by Signature Descriptors and Real Coded Genetic Algorithm
Vikrant A. Dev, Nishanth G. Chemmangattuvalappil, and Mario R. Eden

Coupling Refrigeration System Synthesis and Heat Exchanger Network Design
Ha Dinh and Qiang Xu

Techno-economic Analysis of Production and Recovery of Volatile Fatty Acids from Brown Algae using Membrane Distillation
Peyman Fasahati and Jay Liu

Application of the Generic Modeling Template Approach to Unsaturated Fatty Acid Oxidation and Crystallization Systems
Marina Fedorova, Emmanouil Papadakis, Kresten Troelstrup Meisler, Gürkan Sin, and Rafiqul Gani

The Effect of Stage Recovery Uncertainties on the Selection of Process Structures
Edelmira D. Gálvez and Luis A. Cisternas

Development of QSPR Model Relating Solvent Structure to Crystal Morphology
J. Colin Haser, Robert H. Herring III, Shounak Datta, and Mario R. Eden

Graph-Based Genetic Algorithm for De Novo Molecular Design
Robert H. Herring III and Mario R. Eden

Simulation of Spherical Particle Breakage
Priscilla J. Hill

Solution Strategies to Stochastic Design of Mineral Flotation Plants
Nathalie Jamett, Luis Cisternas, and Juan Pablo Vielma

Bayesian Estimation, Uncertainty Propagation, and Design of Experiments for CO2 Adsorption on Amine Sorbents
Jayashree Kalyanaraman, Yoshiaki Kawajiri, and Matthew Realff

Feasible Design of Multi-component Heterogeneous Reactive Distillation
Dohyung Kang and Jae W. Lee

Computer-aided Molecular Design of ORC Working Fluids using PC-SAFT
Matthias Lampe, Christoph Kirmse, Elamar Sauer, Marina Stavrou, Joachim Gross, and André Bardow

Static and Dynamic Simulation of NOx Absorption Tower Based on a Hybrid Kinetic-Equilibrium Reaction Model
Yunda Liu, David Bluck, and Francisco Brana-Mulero

New Perspective on Computer Aided Molecular Design: a Life Cycle Assessment Approach
Amirhossein Mehrkesh and Arunprakash T. Karunanithi

Uncertainty Quantification in Pharmaceutical Development
Linas Mockus, David LeBlond, and Gintaras V. Reklaitis

Mathematical Programming Shortcut Screening Models for the Design of Integrated Waste Treatment Systems
Athanassios Nikolakopoulos, Lazarus Thomaidis, and Antonis Kokossis

Robust Chemical Product Design via Fuzzy Optimisation Approach
Lik Yin Ng, Nishanth G. Chemmangattuvalappil, and Denny K.S. Ng

Optimal Design of Air Separation Plants with Variable Electricity Pricing
Richard C. Pattison and Michael Baldea

Robust Autothermal Microchannel Reactors
Richard C. Pattison and Michael Baldea

Effect of Ship Tilting on Amine Absorber with Structured-packing for CO2 Removal from Natural Gas
Dung A. Pham,Young-Il Lim, Hyunwoo Jee, Kwangjoon Min, Youngwon Jung, and Sun-Keun Lee

A General Methodology for Energy Efficiency of Industrial Chemical Processes
Nasibeh Pouransari, Mathilde Mercier, Guy-Noel Sauvion, and François Maréchal

Systematic and Optimization-Based Design of Integrated Reaction-Separation Processes
Sebastian Recker, Mirko Skiborowski, Christian Redepenning, and Wolfgang Marquardt

A Systematic Methodology Based on Residue Curve Maps for the Design of Batch Distillation Processes
Alicia Román-Martínez, Ilse de Jesus Nava-Juárez, Marco Tulio Gallo-Estrada, Raúl González-García, and Pedro Antonio Alonso-Dávila

Considering Parameter Uncertainties in the Design of Safe Processes
Mordechai Shacham and Neima Brauner

Conceptual Design and Optimisation of Chemical Processes under Uncertainty by Two-Stage Programming
Jochen Steimel and Sebastian Engell

Designing Optimum Protein-Excipient Interactions using Molecular Docking Simulations
Haider S. Tarar, Brock C. Roughton, and Kyle V. Camarda

Process Modeling - Enabling Sustainable & Economically Attractive Innovation
Stephen M. Tieri, Bruce M. Vrana, Steven L. Grise, Donald E. McConnell, and David W. Drew

Process Synthesis, Design and Analysis using Process-Group Contribution Method
Anjan K. Tula, Mario R. Eden, and Rafiqul Gani

Investigation of Process Efficiency of an Indirectly Heated Solar Reformer
Henrik von Storch, Martin Roeb, Hannes Stadler, and Robert Pitz-Paal

Attainable Regions in Crystallization Processes: Their Construction and the Influence of Parameter Uncertainty
Thomas Vetter, Christopher L. Burcham, and Michael F. Doherty

Systematic Chemical Reaction Pathway Synthesis for Sustainable Integrated Biorefineries
Viknesh Andiappan, Lik Yin Ng, Nishanth G. Chemmangattuvalappil, and Denny K. S. Ng

Simultaneous Optimization and Heat Integration Based on Rigorous Process Simulations
Yang Chen, John Eslick, Ignacio Grossmann and David Miller

Nitrogen- and Climate Impact-based Metrics in Biomass Supply Chains
Lidija Čuček, Jiří J. Klemeš, and Zdravko Kravanja

Early Stage Design of a Biorefinery from Castor Oil
Daniela de Faria, Alberto Quaglia, Fernando L.P. Pessoa, and Rafiqul Gani

Self-sufficient Integrated Algae Based Facility for Diesel Substitutes: FAEE and Glycerol Ethers
Verónica de la Cruz, Sara Hernández, Mariano Martín, and Ignacio E. Grossmann

Equation-Oriented Optimization of Cryogenic Systems for Coal Oxycombustion Powerplants
Alexander W. Dowling, Qianwen Gao and Lorenz T. Biegler

Industrial-scale Bioethanol Production from Brown Algae and Economic Comparison of Two Pretreatment Designs
Peyman Fasahati and Jay Liu

Multi-scale Material Screening and Process Optimization for Natural Gas Purification
Eric L. First, M. M. Faruque Hasan, and Christodoulos A. Floudas

Optimal Integration of Compression Heat with Regenerative Steam Rankine Cycles
Chao Fu, Rahul Anantharaman, and Truls Gundersen

Synergistic Biomass and Natural Gas Conversion to Liquid Fuel with Reduced CO2 Emissions
Emre Gencer, Dharik Mallapragada, Mohit Tawarmalani, and Rakesh Agrawal

MINLP Model and Algorithm for Superstructure Optimization of Algae Processing Network
Jian Gong and Fengqi You

Making Transportation Fuels and Electricity from Non-petroleum-based Hybrid Processes: Process Design and Optimization
Chang He and Fengqi You

Environmental Impact Assessment of Biorefinery Products Using Life Cycle Analysis
Paraskevi Karka, Stavros Papadokonstantakis, Konrad Hungerbühler, and Antonis Kokossis

A Mathematical Decomposition for the Synthesis and the Application of Total Site Analysis on Multiproduct Biorefineries
Dimitrios Koufolioulios, Athanassios Nikolakopoulos, Konstantinos Pyrgakis, and Antonis Kokossis

Application of Process Systems Engineering (PSE) Tools in Designing the Biorefinery
Behrang Mansoornejad, Shabnam Sanaei, Banafsheh Gilani, Marzouk Benali, and Paul Stuart

Current Status of Optimal Design of Natural Gas Liquefaction Process
Il Moon, Inkyu Lee, Kyungjae Tak, Sunkyu Lee, and Daeho Ko

Design and Optimisation of Power Plant Utility Systems
Mkhokheli Ndlovu and Thokozani Majozi

Production of Liquid Transportation Fuels From Coal and Duckweed Biomass
Alexander M. Niziolek, Onur Onel, Josephine A. Elia, Christodoulos A. Floudas, and Xin Xiao

Multi-objective Design of Industrial Symbiosis in Palm Oil Industry
Rex T. L. Ng, Mimi H. Hassim, Denny K. S. Ng, Raymond R. Tan, and Mahmoud M. El-Halwagi

Carbon Constrained Energy Planning (CCEP) with Carbon Capture and Storage Incorporating Carbon Credit Exchange
Raymond E. H. Ooi and Dominic C. Y. Foo

Design Analysis of Integrated Microalgae Biorefineries
Melina Psycha, Kostantinos Pyrgakis, Patricia J. Harvey, Ami Ben-Amotz, A. Keith Cowan, and Antonis Kokossis

A Methodology for the Optimization of Bioethanol Production via Biochemical Pathways
Jonathan P. Raftery and M. Nazmul Karim

Shale Gas for the Petrochemical Industry: Incorporation of Novel Technologies
Yaser Khojasteh Salkuyeh and Thomas A. Adams II

Designing a Waste to Energy Plant for Informal Settlements
Baraka C. Sempuga, Diane Hildebrandt, David Glasser, and Mohamed Seedat

Synthesis of Catalytic Biomass-to-Fuels Strategies
S. Murat Sen, Jeehoon Han, Jeremy S. Luterbacher, David Martin Alonso, James A. Dumesic, and Christos T. Maravelias

Screening and Assessing Product Portfolios in Biorefineries Combining Total Site Analysis and Process Synthesis
Michail E. Stefanakis, Konstantinos A. Pyrgakis, and Antonis C. Kokossis

A Novel Model for Evaluating the Viability of Strategies for Biorefining Processes from Various Stakeholder Perspectives: Case Study on Marginal Land Utilization
Sumesh Sukumara and Jeffrey R. Seay

Optimization and Heat Integration of Hollow Fiber based Thermal Swing Adsorption Process for CO2 Capture from Flue Gas
Subramanian Swernath, Fateme Rezaei, Jayashree Kalyanaraman, Ryan P. Lively, Matthew J. Realff, and Yoshiaki Kawajiri

Modeling and Simulating Electrochemical Reduction of CO2 in a Microfluidic Cell
Kunna Wu, Erik Birgersson, Paul J. A. Kenis, and Iftekhar A. Karimi

Two Stage Bilevel Programming Approach for Representation of Biorefinery Investment Decision Making in a Pre-Established Timberlands Supply Chain
Kevin Yeh, Jay H. Lee, Craig Whittaker, and Matthew J. Realff

Functional-Unit-Based Life Cycle Optimization of Sustainable Biomass-to-Electricity Supply Chain with Economic and Environmental Tradeoffs
Dajun Yue and Fengqi You

Design of Combined Heat and Power Microgrids
Michael Zachar, Milana Trifkovic, and Prodromos Daoutidis

Forecastability as a Design Criterion in Wind Resource Assessment
Jie Zhang and Bri-Mathias Hodge

GLOBIE: An Algorithm for the Deterministic Global Optimization of Box-constrained NLPs
Nikolaos Kazazakis and Claire S. Adjiman

A Parallel Spectral-Projected-Gradient Method for Optimization in Process Engineering
Juan Ignacio Ardenghi, Gustavo Esteban Vazquez, and Nélida Beatriz Brignole

Rigorous Incorporation of Phase Equilibrium Calculations in Pressure Flow Networks for Plant Scale Dynamic Simulation
Ian Boys

Application of Self-tuning High-fidelity Dynamic Simulation Model for Soft-sensing
Abhisek Roy Chowdhary

MOSAIC: An Online Modeling Platform Supporting Automatic Discretization of Partial Differential Equation Systems
Erik Esche, David Müller, Gregor Tolksdorf, Robert Kraus, and Günter Wozny

Systematic Modeling for Optimization
Erik Esche, David Müller, and Günter Wozny

Parallel Solution of Nonlinear Contingency-constrained Network Problems
Jia Kang, John D. Siirola, and Carl D. Laird

Natural Language Modelling in Process Synthesis and Optimization
Vassilis Magioglou, Marinella Tsakalova, and Antonis Kokossis

Systematic Parameter Selection for Optimization under Uncertainty
David Müller, Erik Esche, Diana C. Lopez C., and Günter Wozny

Indicators of Social Sustainability for Wastewater Treatment Processes
Tamara Popovic, Andrzej Kraslawski, René Heiduschke, and Jens-Uwe Repke

Visual Modelling
Heinz A Preisig

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