

# FOCAPD 2009

## Foundations of Computer-Aided Process Design

June 7 – June 12, 2009 ♦ Beaver Run Resort ♦ Breckenridge, Colorado

TENTATIVE FINAL

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### Sunday, June 7

7:00 a.m. to	9:00 a.m.	Workshop Registration
8:30 a.m. to	10:15 a.m.	<b>Workshop on Teaching Product and Process Design</b> <i>Warren Seider, University of Pennsylvania</i> <i>Soemantri Widagdo, 3M Corporation</i>
<b>10:15 a.m. to</b>	<b>10:30 a.m.</b>	<b>Refreshment Break</b>
10:30 a.m. to	12:00 p.m.	Workshop on Teaching Product and Process Design (cont'd)
<b>12:00 p.m. to</b>	<b>1:15 p.m.</b>	<b>Lunch on own</b>
1:15 p.m. to	3:00 p.m.	Workshop on Teaching Product and Process Design (cont'd)
<b>3:00 p.m. to</b>	<b>3:15 p.m.</b>	<b>Refreshment Break</b>
3:15 p.m. to	4:30 p.m.	Workshop on Teaching Product and Process Design (cont'd)
	4:30 p.m.	Workshop concludes

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1:00 p.m. to	7:00 p.m.	Conference Registration
<b>6:00 p.m. to</b>	<b>7:30 p.m.</b>	<b>Welcome Reception</b>
<b>7:30 p.m. to</b>	<b>7:45 p.m.</b>	<b>Welcome Address</b> Conference Chairs: <i>Andreas Linninger, University of Illinois at Chicago</i> <i>Mahmoud El-Halwaghi, Texas A&amp;M University</i>
<b>7:45 p.m. to</b>	<b>9:00 p.m.</b>	<b>Keynote Address</b> Sustainability – What Does it Mean in Practice? <i>Beth Beloff, Sustainable Insight LLC</i>
9:00 p.m. to	11:00 p.m.	Hospitality

## Monday, June 8

7:00 a.m. to	5:00 p.m.	Conference Registration
7:00 a.m. to	8:00 a.m.	Continental Breakfast
<b>8:00 a.m. to</b>	<b>11:30 a.m.</b>	<b>ENERGY SYSTEMS DESIGN AND ALTERNATIVE ENERGY SOURCES</b> <i>Chair: Luke Achenie, Virginia Tech University</i> <i>Co-Chair: Gavin Towler, UOP</i>
8:00 a.m. to	8:45 a.m.	Transportation Fuel in a Solar Economy <i>Rakesh Agrawal, Purdue University</i>
8:45 a.m. to	9:30 a.m.	“The Emerald Forest” – An Integrated Approach for Sustainable Community Development and Bio-derived Energy Generation <i>Fouad Teymour, Illinois Institute of Technology</i>
<b>9:30 a.m. to</b>	<b>10:00 a.m.</b>	<b>Refreshment Break</b>
10:00 a.m. to	10:45 a.m.	Dynamic Optimisation and Multi-parametric Model Predictive Control of Hydrogen Desorption in Metal-hydride Bed <i>Konstantinos Kouramas, Imperial College London</i>
10:45 a.m. to	11:30 a.m.	Panel Discussion
<b>11:30 a.m. to</b>	<b>2:00 p.m.</b>	<b>Lunch on own</b>
<b>2:00 p.m. to</b>	<b>5:00 p.m.</b>	<b>DESIGN FOR SUSTAINABILITY AND ENERGY EFFICIENCY</b> <i>Chair: Rafiqul Gani, Technical University of Denmark</i> <i>Co-Chair: Bhavik Bakshi, Ohio State University</i>
2:00 p.m. to	2:45 p.m.	Molecular Structure Based Short-Cut Models to Retrieve Cradle-to-Gate Aggregated Energy Data for Basic and Specialty Chemicals <i>Konrad Hungerbühler, Swiss Federal Institute of Technology, Zurich</i>
2:45 p.m. to	3:30 p.m.	Embedding Sustainability into Process Development: GlaxoSmithKline's Experiences <i>Concepción Jiménez-González, GlaxoSmithKline</i>
<b>3:30 p.m. to</b>	<b>3:45 p.m.</b>	<b>Refreshment Break</b>
3:45 p.m. to	4:30 p.m.	Green Process Design, Green Energy, and Sustainability: A Systems Analysis Perspective <i>Urmila Diwekar, Vishwamitra Research Institute</i>
4:30 p.m. to	5:00 p.m.	Panel Discussion
<b>5:00 p.m. to</b>	<b>6:30 p.m.</b>	<b>Dinner on own</b>
<b>6:30 p.m. to</b>	<b>9:30 p.m.</b>	<b>ROBUST AND UNCERTAIN SYSTEMS</b> <i>Chair: Mark Stadtherr, Notre Dame University</i> <i>Co-Chair: Chau-Chyun Chen, AspenTech</i>
6:30 p.m. to	7:15 p.m.	Scope for the Application of Mathematical Programming Techniques in the Synthesis and Design of Sustainable Processes <i>Ignacio Grossmann, Carnegie Mellon University</i>
7:15 p.m. to	8:00 p.m.	Rigorous Propagation of Imprecise Probabilities in Process Models <i>Mark Stadtherr, Notre Dame University</i>
8:00 p.m. to	8:15 p.m.	<b>Refreshment Break</b>

8:15 p.m. to	9:00 p.m.	Are Mechanistic Cellulose-Hydrolysis Models Reliable for Use in Biofuel Process Design? Identifiability and Sensitivity Analysis <i>Gürkan Sin, Technical University of Denmark</i>
9:00 p.m. to	9:30 p.m.	Panel Discussion
9:30 p.m. to	11:00 p.m.	Hospitality

## Tuesday, June 9

7:00 a.m. to	5:00 p.m.	Conference Registration
7:00 a.m. to	8:00 a.m.	Continental Breakfast
<b>8:00 a.m. to</b>	<b>11:30 a.m.</b>	<b>DESIGN OF BIOFUELS, BIOLOGICAL PROCESSES AND BIOREFINERIES</b> <i>Chair: Patrick Linke, Texas A&amp;M University-Qatar</i> <i>Co-Chair: Bruce Vrana, DuPont</i>
8:00 a.m. to	8:40 a.m.	Next Generation Hydrocarbon Biorefineries <i>John Regalbuto, National Science Foundation</i>
8:40 a.m. to	9:20 a.m.	Future System Challenges in the Design of Renewable Energy Systems and the Synthesis of Sustainable Biorefineries <i>Antonis Kokossis, National Technical University of Athens</i>
9:20 a.m. to	10:00 a.m.	Bioethanol Production System in Northern Italy: Supply Chain Design and Cost Optimisation <i>Andrea Zamboni, University of Padova</i>
<b>10:00 a.m. to</b>	<b>10:30 a.m.</b>	<b>Refreshment Break</b>
10:30 a.m. to	11:10 a.m.	Discovery of Novel Routes for the Production of Fuels and Chemicals <i>Linda Broadbelt, Northwestern University</i>
11:10 a.m. to	11:40 a.m.	Panel Discussion
<b>11:40 a.m. to</b>	<b>2:00 p.m.</b>	<b>Lunch on own</b>
2:00 p.m. to	4:00 p.m.	Early afternoon free for discussions and meetings
<b>4:00 p.m. to</b>	<b>6:30 p.m.</b>	<b>EMERGING TECHNOLOGIES AND PROCESSES FOR THE ENVIRONMENT</b> <i>Chair: Paul Stuart, École Polytechnique de Montréal</i> <i>Co-Chair: Claire Adjiman, Imperial College London</i>
4:00 p.m. to	4:40 p.m.	Smart Process Manufacturing: A Vision of the Future <i>Thomas Edgar, University of Texas at Austin</i>
4:40 p.m. to	5:20 p.m.	Designing Sustainable Process Networks by Integration of Industrial and Ecological Systems <i>Bhavik Bakshi, Ohio State University</i>
<b>5:20 p.m. to</b>	<b>5:30 p.m.</b>	<b>Refreshment Break (I think you will need some type of bathroom break here)</b>
5:30 p.m. to	6:10 p.m.	Advanced Co-Simulation for Computer-Aided Process Design and Optimization of Fossil Energy Systems with Carbon Capture <i>Stephen Zitney, National Energy Technology Laboratory</i>
6:10 p.m. to	6:40 p.m.	Panel Discussion
<b>6:40 p.m. to</b>	<b>8:00 p.m.</b>	<b>Dinner on own</b>
<b>8:00 p.m. to</b>	<b>8:30 p.m.</b>	<b>SUMMARY OF POSTER PRESENTATIONS</b>  I. Design for Sustainability and Energy Efficiency <i>Chair: Rafiqul Gani, Technical University of Denmark</i>  II. Emerging Technologies and Processes for the Environment <i>Chair: Paul Stuart, École Polytechnique de Montréal</i>

III. Design of Biofuels, Biological Processes and Biorefineries

*Chair: Patrick Linke, Texas A&M University-Qatar*

IV. Energy Systems Design and Alternative Energy Sources

*Chair: Luke Achenie, Virginia Tech University*

*Co-Chair: Gavin Towler, UOP*

**8:30 p.m. to 10:00 p.m. Poster Session A** (refreshments provided)

## Wednesday, June 10

7:00 a.m. to 7:00 a.m. to	5:00 p.m. 8:00 a.m.	Conference Registration Continental Breakfast
<b>8:00 a.m. to</b>	<b>11:30 a.m.</b>	<b>FUTURE PROCESS DESIGN EDUCATION</b> <i>Chair: Andy Hrymak, McMaster University</i> <i>Co-Chair: Warren Seider, University of Pennsylvania</i>
8:00 a.m. to	8:20 a.m.	Update/Synopsis of the Product Design Workshop <i>Warren Seider, University of Pennsylvania</i>
8:20 a.m. to	9:00 a.m.	Web-Based Modules For Product and Process Design <i>Paul Stuart, École Polytechnique de Montréal</i>
9:00 a.m. to	9:40 a.m.	Undergraduate Education: Robust Design through Operability <i>Thomas Marlin, McMaster University</i>
<b>9:40 a.m. to</b>	<b>10:15 a.m.</b>	<b>Refreshment Break</b>
10:15 a.m. to	10:55 a.m.	Integrating Computer Aided Design Across the Curriculum <i>Gavin Towler, UOP</i>
10:55 a.m. to	11:30 a.m.	Panel Discussion
<b>11:30 a.m. to</b>	<b>12:30 p.m.</b>	<b>Lunch on own</b>
<b>12:30 p.m. to</b>	<b>5:00 p.m.</b>	<b>Breakout Sessions</b> <i>Chair: Dennis Spriggs, Matrix Process Integration</i>
<b>5:00 p.m. to</b>	<b>6:00 p.m.</b>	<b>Reconvene Breakout Sessions</b> <i>Chair: Dennis Spriggs, Matrix Process Integration</i>
<b>6:00 p.m. to</b>	<b>7:30 p.m.</b>	<b>Dinner on own</b>
<b>7:30 p.m. to</b>	<b>8:00 p.m.</b>	<b>SUMMARY OF POSTER PRESENTATIONS</b>
		V. Multi-Scale and Complex Systems <i>Chair: Yannis Kevrekidis, Princeton University</i> <i>Co-Chair: Ipsita Banerjee, University of Pittsburgh</i>
		VI. Robust and Uncertain Systems <i>Chair: Mark Stadtherr, Notre Dame University</i> <i>Co-Chair: Chau-Chyun Chen, AspenTech</i>
		VII. Future Process Design Education <i>Chair: Andy Hrymak, McMaster University</i> <i>Co-Chair: Warren Seider, University of Pennsylvania</i>
		VIII. Emerging Tools and Techniques in Process Design <i>Chair: Mario Eden, Auburn University</i> <i>Co-Chair: Venkat Subramanian, Tennessee Tech University</i>
		IX. Product and Process Design I - Products <i>Chair: Andres Malcolm, Cargill</i> <i>Chair: Carl Laird, Texas A&amp;M University</i>
		X. Product and Process Design II - Processes <i>Chair: Kyle Camarda, University of Kansas</i> <i>Chair: Christos Maravelias, University of Wisconsin – Madison</i>

**8:00 p.m. to 10:00 p.m. Poster Session** (refreshments provided)

## Thursday, June 11

7:00 a.m. to 8:00 a.m. Continental Breakfast

**8:00 a.m. to 11:30 a.m. MULTI-SCALE AND COMPLEX SYSTEMS**  
*Chair: Yannis Kevrekidis, Princeton University*  
*Co-Chair: Ipsita Banerjee, University of Pittsburgh*

8:00 a.m. to 8:40 a.m. Advances In Global Optimization for Standard, Generalized, and Extended Pooling Problems with the (EPA) Complex Emissions Model Constraints  
*Christodoulos Floudas, Princeton University*

8:40 a.m. to 9:20 a.m. Multi-Scale Methods and Complex Processes: A Survey and Look Ahead  
*Angelo Lucia, University of Rhode Island*

**9:20 a.m. to 10:10 a.m. Refreshment Break**

10:10 a.m. to 10:50 a.m. Controlled Formation of Nanostructures with Desired Geometries  
*George Stephanopoulos, MIT*

10:50 a.m. to 11:30 a.m. Tight Energy Integration: Easier Control?  
*Prodromos Daoutidis, University of Minnesota*

11:30 a.m. to 12:00 p.m. Panel Discussion

**12:00 p.m. to 2:00 p.m. Lunch on own**

**2:00 p.m. to 4:00 p.m. PRODUCT AND PROCESS DESIGN I – PRODUCTS**  
*Chair: Andres Malcolm, Cargill*  
*Chair: Carl Laird, Texas A&M University*

2:00 p.m. to 2:40 p.m. Design of Ionic Liquids via Computational Molecular Design  
*Kyle Camarda, University of Kansas*

2:40 p.m. to 3:20 p.m. Biodiesel Process Design through a Computer-aided Molecular Design Approach  
*Arunprakash Karunanithi, University of Colorado Denver*

3:20 p.m. to 4:00 p.m. Model Reformulation and Design of Lithium-Ion Batteries  
*Venkat Subramanian, Tennessee Tech University*

**4:00 p.m. to 4:30 p.m. Refreshment Break**

**4:30 p.m. to 6:30 p.m. PRODUCT AND PROCESS DESIGN II – PROCESSES**  
*Chair: Kyle Camarda, University of Kansas*  
*Chair: Christos Maravelias, University of Wisconsin – Madison*

4:30 p.m. to 5:10 p.m. Computer-Aided Graphical Tools for Synthesizing Complex Column Configurations  
*Diane Hildebrand, University of the Witwatersrand*

5:10 p.m. to 5:50 p.m. Integrating Product Portfolio Design and Supply Chain Design for the Forest Biorefinery  
*Paul Stuart, École Polytechnique - Montréal*

5:50 p.m. to 6:30 p.m. A Novel Shortcut Method for the Design of Heteroazeotropic Distillation of Multicomponent Mixtures  
*Korbinian Kraemer, RWTH Aachen University*

7:00 p.m. to 9:30 p.m. Reception and Banquet

## Friday, June 12

7:00 a.m. to 8:00 a.m. Continental Breakfast

8:00 a.m. to 11:30 a.m. **EMERGING TOOLS AND TECHNIQUES IN PROCESS DESIGN**

*Chair: Mario Eden, Auburn University*

*Co-Chair: Venkat Subramanian, Tennessee Tech University*

8:00 a.m. to 8:40 a.m. Constructing, Modifying and Maintaining Consistent Process Models  
*Heinz Preisig, NTNU, Norway*

8:40 a.m. to 9:20 a.m. Design Under Uncertainty: Chemical Process Plants to Biological Networks  
*Ipsita Banerjee, University of Pittsburgh*

9:20 a.m. to 9:45 a.m. **Refreshment Break**

9:45 a.m. to 10:25 a.m. Mathematical Modeling in Process Design and Operation: Structural Assessment  
*Ferenc Friedler, University of Pannonia, Hungary*

10:25 a.m. to 10:55 a.m. Panel Discussion

10:55 a.m. to 11:30 a.m. Conference Closure and Wrap-up  
*Jeff Sirola, Eastman Chemical*