

FOCAPO / CPC 2023

Grand Challenges

Digitalization ♦ Sustainability ♦ Innovation Speed ♦ Future of PSE

January 8 – January 12, 2023

Hilton San Antonio Hill Country ♦ San Antonio, Texas

FINAL PROGRAM

Sunday, January 8

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| 2:00 p.m. to 8:30 p.m. | Conference Registration (<i>Grand Hallway</i>) |
| 7:30 p.m. to 8:30 p.m. | OPENING SESSION (<i>Oak Ballroom</i>) |
| 7:30 p.m. to 7:45 p.m. | Opening Remarks
<i>Michael Baldea (University of Texas at Austin)</i>
<i>Rahul Bindlish (The Dow Chemical Company)</i>
<i>Iiro Harjunkoski (Hitachi Energy)</i>
<i>Victor Zavala (University of Wisconsin – Madison & Argonne National Lab)</i> |
| 7:45 p.m. to 8:30 p.m. | Opening Plenary
The Quest Towards the Integration of Process Control, Process Operations and Process Operability – Industrial Need or Academic Curiosity?
<i>Stratos Pistikopoulos (Texas A&M University)</i> |
| 8:30 p.m. to 10:00 p.m. | Welcome Reception (<i>Spanish Oaks & Rotunda</i>) |

Monday, January 9 – Joint Session (*Oak Ballroom*)

- 7:00 a.m. to 5:00 p.m.** **Conference Registration** (*Grand Hallway*)
- 7:30 a.m. to 8:30 a.m.** **Continental Breakfast** (*Spurs*)
- 8:30 a.m. to 9:30 a.m.** **PLENARY SESSION – DIGITALIZATION**
Chair: Iiro Harjunkoski (Hitachi Energy)

Power Systems of the Future
Ernst Scholtz and Alexandre Oudalov (Hitachi Energy)
- 9:30 a.m. to 10:00 a.m.** **Refreshment Break**
- 10:00 a.m. to 12:30 p.m.** **KEYNOTE SESSION – DIGITALIZATION**
Chair: Ignacio Grossmann (Carnegie Mellon University)
Chair: Cristiana Lara (Amazon)
- 10:00 a.m. to 10:30 a.m. Cybersecurity in Process Control, Operations and Supply Chains
Panagiotis Christofides (University of California – Los Angeles)
Sandra Parker (The Dow Chemical Company)
- 10:30 a.m. to 11:00 a.m. Formulating Data-driven Surrogate Models for Process Optimization
Ruth Misener (Imperial College London)
Larry Biegler (Carnegie Mellon University)
- 11:00 a.m. to 11:30 a.m. Resilient Manufacturing Ecosystems through Artificial Intelligence
James Davis (University of California – Los Angeles)
- 11:30 a.m. to 12:00 p.m. Impact of Emerging Computing Architectures and Opportunities for
Process Systems Engineering Application
Carl Laird (Carnegie Mellon University)
Stuart Harwood (ExxonMobil)
David Bernal (NASA)
Dimitar Trenev (ExxonMobil)
Davide Venturelli (NASA)
- 12:00 p.m. to 12:30 p.m. Digital Transformation and Expanding the Capabilities of Industrial
Process Control and Optimization
Whit McConnell (ExxonMobil)
Dimitrios Georgis (ExxonMobil)
Tyler Soderstrom (ExxonMobil)
Jitendra Kadam (ExxonMobil)
- 12:30 p.m. to 2:00 p.m.** **Lunch** (*Hill Country Café/Sun Deck*)

Monday, January 9 – Parallel Sessions

ORAL SESSIONS – (Red Oak & Monterey Oak)

- 2:00 p.m. to 3:40 p.m.** **EMERGING TRENDS IN DIGITALIZATION**
Chair: Carl Laird (Carnegie Mellon University)
Chair: Bethany Nicholson (Sandia National Laboratories)
- 2:00 p.m. to 2:25 p.m. Towards a Digital Twin for Analytical HPLC
Monica Tirapelle (University College London)
- 2:25 p.m. to 2:50 p.m. Enhanced CNN with Global Features for Fault Diagnosis of Complex Chemical Processes
Qiugang (Jay) Lu (Texas Tech University)
- 2:50 p.m. to 3:15 p.m. Perspectives on Design Considerations Inspired by Security and Quantum Technology in Cyberphysical Systems for Process Engineering
Helen Durand (Wayne State University)
- 3:15 p.m. to 3:40 p.m. Automatic Source Code Generation of Complicated Models for Deterministic Global Optimization with Parallel Architectures
Matthew Stuber (University of Connecticut)

ORAL SESSIONS – (Live Oak)

- 2:00 p.m. to 3:40 p.m.** **ADVANCES IN MACHINE LEARNING**
Chair: Zheyu Jiang (Oklahoma State University)
Chair: Alexander Smith (University of Minnesota)
- 2:00 p.m. to 2:25 p.m. Learning to Initialize Generalized Benders Decomposition via Active Learning
Ilias Mitrai (University of Minnesota)
- 2:25 p.m. to 2:50 p.m. Optimization-based Approaches for Design of Chemical Process Families using ReLU Surrogates
Georgia Stinchfield (Carnegie Mellon University)
- 2:50 p.m. to 3:15 p.m. Safe Deployment of Reinforcement Learning Using Deterministic Optimization of Trained Neural Networks
Calvin Tsay (Imperial College London)
- 3:15 p.m. to 3:40 p.m. A Gaussian Process Embedded Feature Selection Method Based on Automatic Relevance Determination
Yushi Deng (Auburn University)
- 3:40 p.m. to 4:10 p.m.** **Refreshment Break**

Monday, January 9 – Parallel Sessions (Continued)

ORAL SESSIONS Continued – (Red Oak & Monterey Oak)

- 4:10 p.m. to 5:50 p.m.** **ENERGY SYSTEMS & INFRASTRUCTURE**
Chair: Qi Zhang (University of Minnesota)
Chair: Calvin Tsay (Imperial College London)
- 4:10 p.m. to 4:35 p.m. Towards Optimal Energy-water Supply System Operation for Agricultural and Metropolitan Ecosystems
Marcello Di Martino (Texas A&M University)
- 4:35 p.m. to 5:00 p.m. A Conditional Value-at-Risk Framework for Optimal Microgrid Day-ahead Market Bidding
Robert Herding (University College London)
- 5:00 p.m. to 5:25 p.m. Stochastic Programming of Energy System Operations Considering Terminal Energy Storage Levels
Teemu Ikonen (Aalto University)
- 5:25 p.m. to 5:50 p.m. Opportunities for Industrial Demand Response: A Survey of Grid-responsive Smart Manufacturing Applications
Blake Billings (University of Utah)

ORAL SESSIONS Continued – (Live Oak)

- 4:10 p.m. to 5:50 p.m.** **ADVANCES IN DATA SCIENCE**
Chair: Aaron Liu (Georgia Tech University)
Chair: Wentao Tang (North Carolina State University)
- 4:10 p.m. to 4:35 p.m. Applied Topology and Geometry in Process Monitoring and Fault Detection
Alexander Smith (University of Minnesota)
- 4:35 p.m. to 5:00 p.m. Application of Grey-box Modeling for System Health Monitoring in Manufacturing
Utsav Awasthi (University of Connecticut)
- 5:00 p.m. to 5:25 p.m. Data-based Modeling and Control of Nonlinear Process Systems Using Sparse Identification: An Overview of Recent Results
Panagiotis Christofides (University of California – Los Angeles)
- 5:25 p.m. to 5:50 p.m. Improving Moving Horizon Estimation Using Parametric Nonlinear Programming Sensitivities
Simen Bjorvand (NTNU)
- 5:50 p.m. to 8:00 p.m.** **Free Time & Dinner on Your Own**
- 8:00 p.m. to 10:00 p.m.** **Poster Session A – Digitalization & Innovation Speed (Rotunda)**
Chair: Salvador Garcia Muñoz (Eli Lilly)
Chair: Mona Bavarian (University of Nebraska – Lincoln)

Tuesday, January 10 – Joint Session (*Oak Ballroom*)

- 7:00 a.m. to 5:00 p.m.** **Conference Registration** (*Grand Hallway*)
- 7:30 a.m. to 8:30 a.m.** **Continental Breakfast** (*Spurs*)
- 8:30 a.m. to 9:30 a.m.** **PLENARY SESSION – SUSTAINABILITY**
Chair: Michael Baldea (University of Texas at Austin)
- Continuous Monitoring for Measuring and Mitigating Methane Emissions from Oil and Gas Production Operations
David Allen (University of Texas at Austin)
- 9:30 a.m. to 10:00 a.m.** **Refreshment Break**
- 10:00 a.m. to 12:00 p.m.** **KEYNOTE SESSION – SUSTAINABILITY**
Chair: Marianthi Ierapetritou (University of Delaware)
Chair: Panagiotis Christofides (University of California – Los Angeles)
- 10:00 a.m. to 10:30 a.m. Future of CO₂ Management Systems: Design and Operations
David Miller (NETL)
Jaffer Ghouse (NETL)
Radhakrishna Gooty (NETL)
Ben Omell (NETL)
Joshua Morgan (NETL)
Daison Caballero (NETL)
Miguel Zamarripa (NETL)
Sally Homsy (NETL)
Brandon Paul (NETL)
Anuja Deshpande (NETL)
- 10:30 a.m. to 11:00 a.m. Integration of Chemical Process Operation with Energy and Systems Infrastructure
Jesus Flores-Cerrilo (Linde)
Christopher Swartz (McMaster University)
- 11:00 a.m. to 11:30 a.m. Circular Economy Definitions, Challenges and Opportunities
Styliani Avraamidou (University of Wisconsin – Madison)
Ana Torres (Carnegie Mellon University)
- 11:30 a.m. to 12:00 p.m. Systems Engineering for Sustainability in a Globalized World: Resources, Ecosystems, Boundaries
Bhavik Bakshi (The Ohio State University)
Christos Maravelias (Princeton University)
- 12:00 p.m. to 2:00 p.m.** **Lunch** (*Hill Country Café/Sun Deck*)

Tuesday, January 10 – Parallel Sessions

ORAL SESSIONS – (*Red Oak & Monterey Oak*)

- 2:00 p.m. to 3:40 p.m.** **MODELING FOR SUSTAINABILITY**
Chair: Styliana Avraamidou (University of Wisconsin – Madison)
Chair: Matthew Stuber (University of Connecticut)
- 2:00 p.m. to 2:25 p.m. Real-time Characterization of Mixed Plastic Waste Using Machine Learning and Infrared Spectroscopy
Shengli Jiang (University of Wisconsin – Madison)
- 2:25 p.m. to 2:50 p.m. Bridging the Scales from Catalyst Synthesis to Sustainable Process: CO₂ Hydrogenation to Methanol
Lukas Spiekermann (ETH – Zurich)
- 2:50 p.m. to 3:15 p.m. Absolute Life Cycle Optimization of the CDR-Power Nexus
Valentina Negri (ETH – Zurich)
- 3:15 p.m. to 3:40 p.m. A Data-driven Random Walk Approach for Solving Water Flow Dynamics in Soil Systems
Zeyuan Song (Oklahoma State University)

ORAL SESSIONS – (*Live Oak*)

- 2:00 p.m. to 3:40 p.m.** **ADVANCES IN CONTROL**
Chair: Qiugang (Jay) Lu (Texas Tech University)
Chair: Tyler Soderstrom (ExxonMobil)
- 2:00 p.m. to 2:25 p.m. Data-driven Model Reduction and Nonlinear Model Predictive Control of an Air Separation Unit by Applied Koopman Theory
Jan Schulze (RWTH Aachen University)
- 2:25 p.m. to 2:50 p.m. An Industrial Case Study on the Combined Identification and Offset-free Model Predictive Control of a Chemical Process
Steven Kuntz (University of California – Santa Barbara)
- 2:50 p.m. to 3:15 p.m. Automatic Decomposition of Large-scale Industrial Processes for Distributed MPC on the Shell-Yokogawa Platform for Advanced Control and Estimation (PACE)
Wentao Tang (Shell Global Solutions (U.S.) Inc. & NCSU)
- 3:15 p.m. to 3:40 p.m. Handling Interactive Systems in Primal-dual Feedback-optimizing Control
Risvan Dirza (NTNU)
- 3:40 p.m. to 4:10 p.m.** **Refreshment Break**

Tuesday, January 10 – Parallel Sessions (Continued)

ORAL SESSIONS Continued – (Red Oak & Monterey Oak)

- 4:10 p.m. to 5:50 p.m.** **DECARBONIZATION**
Chair: David Miller (NETL)
Chair: George Bollas (University of Connecticut)
- 4:10 p.m. to 4:35 p.m. Co-optimizing Design and Operation Strategy of Solid Oxide Fuel Cell-based Hydrogen-electricity Coproduction Systems
Alexander Dowling (University of Notre Dame)
- 4:35 p.m. to 5:00 p.m. Carbon Emission Trading on The Blockchain: A Game-theoretic Framework
M.M. Faruque Hasan (Texas A&M University)
- 5:00 p.m. to 5:25 p.m. A Multiperiod Model for Portfolio Optimization of Carbon Capture and Utilization
Pooja Zen Santhamoorthy (Auburn University)
- 5:25 p.m. to 5:50 p.m. Simultaneous Design and Operational Optimization Under Uncertainty for Flexible Carbon Capture Plants
Michael Baldea (University of Texas at Austin)

ORAL SESSIONS Continued – (Live Oak)

- 4:10 p.m. to 5:50 p.m.** **DYNAMICS & CONTROL FOR SUSTAINABILITY**
Chair: Helen Durand (Wayne University)
Chair: Yuhe Tian (West Virginia University)
- 4:10 p.m. to 4:35 p.m. An Application of the Dulmage-Mendelsohn Partition to the Analysis of a Discretized Dynamic Chemical Looping Reactor Model
Robert Parker (Carnegie Mellon University)
- 4:35 p.m. to 5:00 p.m. NMPC for Setpoint Tracking Operation of a Solid Oxide Electrolysis Cell System
Douglas Allan (NETL)
- 5:00 p.m. to 5:25 p.m. Dynamic Objective Correlation in Many-objective Optimal Operation: An Ammonia Production Case Study
Andrew Allman (University of Michigan)
- 5:25 p.m. to 5:50 p.m. A Modeling and Closed-loop Planning Strategy to Achieve Net-zero Energy Use in Buildings
Michael Risbeck (Johnson Controls)
- 5:50 p.m. to 6:45 p.m.** **Free Time**
- 6:45 p.m. to 7:30 p.m.** **Conference Reception (Rotunda)**
- 7:30 p.m. to 10:30 p.m.** **Plenary and Conference Banquet (Oak Ballroom)**
- 7:30 p.m. to 7:40 p.m. **Opening Remarks**
Victor Zavala (University of Wisconsin – Madison & Argonne National Lab)
- 7:40 p.m. to 8:30 p.m. **Plenary Presentation**
Harmonizing the Use of Optimization and Feedback in Process Operations and Control
James Rawlings (University of California – Santa Barbara)
- 8:30 p.m. to 10:00 p.m.** **Conference Banquet (Oak Ballroom)**

Wednesday, January 11 – Joint Session *(Oak Ballroom)*

- 7:00 a.m. to 5:00 p.m.** **Conference Registration** *(Grand Hallway)*
- 7:30 a.m. to 8:30 a.m.** **Continental Breakfast** *(Spurs)*
- 8:30 a.m. to 9:30 a.m.** **PLENARY SESSION – INNOVATION SPEED**
Chair: Rahul Bindlish (The Dow Chemical Company)
- Innovating for Speed, Complexity and Sustainability in Pharmaceutical Development and Manufacturing
Celia Cruz (Eli Lilly)
- 9:30 a.m. to 10:00 a.m.** **Refreshment Break**
- 10:00 a.m. to 12:00 p.m.** **KEYNOTE SESSION – INNOVATION SPEED**
Chair: Ruth Misener (Imperial College London)
Chair: Dimitri Papageorgiou (ExxonMobil)
- 10:00 a.m. to 10:30 a.m. Digital Innovation Challenges in the Pharmaceutical Industry
Cleo Kontoravdi (Imperial College London)
Salvador García Muñoz (Eli Lilly)
- 10:30 a.m. to 11:00 a.m. Open-Source Modeling Platforms
John Hedengren (Brigham Young University)
Bethany Nicholson (Sandia National Laboratories)
- 11:00 a.m. to 11:30 a.m. Resilient Supply Chains – Robustness and Dynamics in Global Supply Chains
Jose Pinto (Linde Digital)
Ana Barbosa-Povoa (University of Lisbon)
- 11:30 a.m. to 12:00 p.m. Feasibility/Flexibility-based Optimization for Process Design and Operations
Marianthi Ierapetrirou (University of Delaware)
Huayu Tian (University of Delaware)
Jnana Sai Jagana (University of Minnesota)
Qi Zhang (University of Minnesota)
- 12:00 p.m. to 2:00 p.m.** **Lunch** *(Hill Country Café/Sun Deck)*

Wednesday, January 11 – Parallel Sessions

ORAL SESSIONS – (Red Oak & Monterey Oak)

- 2:00 p.m. to 3:40 p.m.** **MARKETS & LONG-TERM PLANNING**
Chair: Christopher Swartz (McMaster University)
Chair: Andrew Allman (University of Michigan)
- 2:00 p.m. to 2:25 p.m. Data-driven Distributionally Robust Optimization for Long-term Contract vs. Spot Allocation Decisions
Dimitri Papageorgiou (ExxonMobil)
- 2:25 p.m. to 2:50 p.m. Multi-period Fair Customer Allocation in Oligopolies
Asimina Marousi (University College London)
- 2:50 p.m. to 3:15 p.m. Efficient Multi-echelon Inventory Optimization Models for Industrial Practice
Victoria Achkar (Universidad Nacional del Litoral)
- 3:15 p.m. to 3:40 p.m. Bilevel Optimization of Energy System Transition Pathways Considering Competition in Markets
David Yang Shu (ETH Zürich)

ORAL SESSIONS – (Live Oak)

- 2:00 p.m. to 3:40 p.m.** **DATA-DRIVEN CONTROL**
Chair: Joel Paulson (The Ohio State University)
Chair: Michael Risbeck (Johnson Controls)
- 2:00 p.m. to 2:25 p.m. Shared Parameter Network: An Efficient Process Monitoring Model
Lucky Yerimah (Rensselaer Polytechnic Institute)
- 2:25 p.m. to 2:50 p.m. A Risk-Based Reinforcement Learning Algorithm to Improve Acute Renal Replacement Therapy
Robert Parker (University of Pittsburgh)
- 2:50 p.m. to 3:15 p.m. Dynamic Risk-based Design and Explicit Model Predictive Control via Multi-parametric Programming
Yuhe Tian (West Virginia University)
- 3:15 p.m. to 3:40 p.m. Seamless Implementation of a Novel Valves Stiction Detection Algorithm Using Seeq Data Lab
Ashwin Venkat (Seeq Corporation)
- 3:40 p.m. to 4:10 p.m.** **Refreshment Break**

Wednesday, January 11 – Parallel Sessions (Continued)

ORAL SESSIONS Continued – (Red Oak & Monterey Oak)

- 4:10 p.m. to 5:50 p.m.** **FLEXIBILITY & RESILIENCE**
Chair: Ana Torres (Carnegie Mellon University)
Chair: Yankai Cao (University of British Columbia)
- 4:10 p.m. to 4:35 p.m. Surrogate-based Optimization of a Flexible Integrated Biorefinery
Yuqing Luo (University of Delaware)
- 4:35 p.m. to 5:00 p.m. Characterizing Event Constraints with Generalized Disjunctive Programming
Joshua Pulsipher (Carnegie Mellon University)
- 5:00 p.m. to 5:25 p.m. Operation Optimization of Supply Chain Networks Under Disruptions
Daniel Ovalle Varela (Carnegie Mellon University)
- 5:25 p.m. to 5:50 p.m. A Bayesian Optimization Approach for Data-efficient Flexibility Analysis of Expensive Black-box Models
Joel Paulson (The Ohio State University)

ORAL SESSIONS Continued – (Live Oak)

- 4:10 p.m. to 5:50 p.m.** **ADVANCES IN OPTIMIZATION**
Chair: Faruque Hasan (Texas A&M University)
Chair: Kamil Khan (McMaster University)
- 4:10 p.m. to 4:35 p.m. Oil Production Under Gas-coning Conditions by Well-cycling and Mixed-integer Programming
Jose Santiago Rodriguez (ExxonMobil)
- 4:35 p.m. to 5:00 p.m. Computational Performance of Algebraic Modeling Languages with Alternate Solver Interfaces and Advanced Modeling Components
Bashar Ammari (Carnegie Mellon University)
- 5:00 p.m. to 5:25 p.m. Recent Advances in Discrete Time Chemical Production Scheduling MILP Models
Nathan Adalgren (Princeton University)
- 5:25 p.m. to 5:50 p.m. Implementing Adjoint Subgradient Evaluation for Use in Global Dynamic Optimization
Kamil Khan (McMaster University)
- 5:50 p.m. to 8:00 p.m.** **Free Time & Dinner on Your Own**
- 8:00 p.m. to 10:00 p.m.** **Poster Session B – Energy & Sustainability (Rotunda)**
Chair: Kirti Yenkie (Rowan University)
Chair: Jose Santiago Rodriguez (ExxonMobil)

Thursday, January 12 – Joint Session *(Oak Ballroom)*

- 7:30 a.m. to 8:30 a.m.** **Continental Breakfast** *(Spurs)*
- 8:30 a.m. to 9:30 a.m.** **PLENARY SESSION – FUTURE OF PSE**
Chair: Victor Zavala (University of Wisconsin – Madison & Argonne National Lab)
- Developing Strategies for Polymer Redesign and Recycling Using Reaction Pathway Analysis
Linda Broadbelt (Northwestern University)
- 9:30 a.m. to 10:00 a.m.** **Refreshment Break**
- 10:00 a.m. to 12:00 p.m.** **KEYNOTE SESSION – FUTURE OF PSE**
Chair: John Hedengren (Brigham Young University)
Chair: Selen Cremaschi (Auburn University)
- 10:00 a.m. to 10:30 a.m. Hyperscale Modeling: Molecule, Process, Enterprise
Ignacio Grossmann (Carnegie Mellon University)
André Bardow (ETH Zurich)
- 10:30 a.m. to 11:00 a.m. Process Operations: From Models and Data to Digital Applications
Costas Pantelides (Siemens PSE, Inc. & Imperial College London)
Nina Thornhill (Imperial College London)
Frances Pereira (Siemens PSE, Inc.)
Penelope Stanger (Imperial College London)
- 11:00 a.m. to 11:30 a.m. The Future of Control Process Systems
Prodromos Daoutidis (University of Minnesota)
Larry Megan (Baldwin Richardson Foods)
Wentao Tang (North Carolina State University)
- 11:30 a.m. to 12:00 p.m. Future of Supply Chains: Challenges, Trends and Prospects
Cristiana Lara (Amazon)
- 12:00 p.m. to 1:30 p.m.** **Lunch** *(Hill Country Café/Sun Deck)*
- 1:30 p.m. to 3:30 p.m.** **Panel Discussion** *(Oak Ballroom)*
- Summary & Perspectives from FOCAPO/CPC
Costas Pantelides (Siemens PSE, Inc. & Imperial College London)
Ruth Misener (Imperial College London)
Larry Biegler (Carnegie Mellon University)
- 3:30 p.m.** **Conference Concludes**