FOCAPO / CPC 2023

Grand ChallengesDigitalization • Sustainability • Innovation Speed • Future of PSE

January 8 – January 12, 2023

Hilton San Antonio Hill Country ◆ San Antonio, Texas

FINAL PROGRAM

Sunday, January 8

2:00 p.m. to 8:30 p.m. Conference Registration (Grand Hallway)

7:30 p.m. to 8:30 p.m. OPENING SESSION (Red Oak, Monterey Oak & Live Oak)

7:30 p.m. to 7:45 p.m. **Opening Remarks**

Michael Baldea (University of Texas at Austin) Rahul Bindlish (The Dow Chemical Company)

Iiro Harjunkoski (Hitachi Energy)

Victor Zavala (University of Wisconsin – Madison & Argonne National Lab)

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?

Stratos Pistikopoulos (Texas A&M University)

8:30 p.m. to 10:00 p.m. Welcome Reception (Spanish Oaks)

Monday, January 9 – Joint Session (Red Oak, Monterey Oak & Live Oak)

7:00 a.m. to 5:00 p.m. Conference Registration (Grand Hallway)

7:30 a.m. to 8:30 a.m. Continental Breakfast (The Spurs or Spanish Oaks)

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 & The Spurs)

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 <i>Qiugang (Jay) Lu (Texas Tech University)</i>
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 García Muñoz (Eli Lilly) Chair: Mona Bavarian (University of Nebraska – Lincoln)

Tuesday, January 10 – Joint Session (Red Oak, Monterey Oak & Live Oak)

7:00 a.m. to 5:00 p.m. Conference Registration (Grand Hallway)

7:30 a.m. to 8:30 a.m. Continental Breakfast (The Spurs or Spanish Oaks)

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 & The Spurs)

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: CO ₂ 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 Nicole Cortes (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)

Simultaneous Design and Operational Optimization Under

Uncertainty for Flexible Carbon Capture Plants

Michael Baldea (University of Texas at Austin)

ORAL SESSIONS Continued – (Live Oak)

5:25 p.m. to 5:50 p.m.

8:30 p.m. to 10:00 p.m.

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
7:30 p.m. to 10:30 p.m.	Plenary and Conference Banquet (Red Oak, Monterey Oak & Live Oak)
7:30 p.m. to 7:44 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)

Conference Banquet

Wednesday, January 11 – Joint Session (Red Oak, Monterey Oak & Live Oak)

7:00 a.m. to 5:00 p.m. Conference Registration (Grand Hallway)

7:30 a.m. to 8:30 a.m. Continental Breakfast (The Spurs or Spanish Oaks)

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) Oi Zhang (University of Minnesota)

12:00 p.m. to 2:00 p.m. Lunch (Hill Country Café and The Spurs)

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 Litorial)
3:15 p.m. to 3:40 p.m.	Bilevel Optimization of Energy System Transition Pathways Considering Competition in Markets David Yang Shu (ETH Zurich)

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 Adelgren (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 (Red Oak, Monterey Oak & Live Oak)

7:30 a.m. to 8:30 a.m. Continental Breakfast (The Spurs or Spanish Oaks)

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 & The Spurs)

1:30 p.m. to 3:30 p.m. Panel Discussion (Red Oak, Monterey Oak & Live Oak)

3:30 p.m. Conference Concludes