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

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)
  Cybersecurity in Process Control, Operations and Supply Chains
    Panagiotis Christofides (University of California – Los Angeles)
    Sandra Parker (The Dow Chemical Company)
  Formulating Data-driven Surrogate Models for Process Optimization
    Ruth Misener (Imperial College London)
    Larry Biegler (Carnegie Mellon University)
  Resilient Manufacturing Ecosystems through Artificial Intelligence
    James Davis (University of California – Los Angeles)
  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)
  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)*

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Chair 1</th>
<th>Chair 2</th>
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<tbody>
<tr>
<td>2:00 p.m. to 3:40 p.m.</td>
<td><strong>EMERGING TRENDS IN DIGITALIZATION</strong></td>
<td>Carl Laird (Carnegie Mellon University)</td>
<td>Bethany Nicholson (Sandia National Laboratories)</td>
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<tr>
<td>2:00 p.m. to 2:25 p.m.</td>
<td>Towards a Digital Twin for Analytical HPLC</td>
<td>Monica Tirapelle (University College London)</td>
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<tr>
<td>2:25 p.m. to 2:50 p.m.</td>
<td>Enhanced CNN with Global Features for Fault Diagnosis of Complex Chemical Processes</td>
<td>Qiugang (Jay) Lu (Texas Tech University)</td>
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<tr>
<td>2:50 p.m. to 3:15 p.m.</td>
<td>Perspectives on Design Considerations Inspired by Security and Quantum Technology in Cyberphysical Systems for Process Engineering</td>
<td>Helen Durand (Wayne State University)</td>
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<tr>
<td>3:15 p.m. to 3:40 p.m.</td>
<td>Automatic Source Code Generation of Complicated Models for Deterministic Global Optimization with Parallel Architectures</td>
<td>Matthew Stuber (University of Connecticut)</td>
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**ORAL SESSIONS** – *(Live Oak)*

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Chair 1</th>
<th>Chair 2</th>
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<tr>
<td>2:00 p.m. to 3:40 p.m.</td>
<td><strong>ADVANCES IN MACHINE LEARNING</strong></td>
<td>Zheyu Jiang (Oklahoma State University)</td>
<td>Alexander Smith (University of Minnesota)</td>
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<tr>
<td>2:00 p.m. to 2:25 p.m.</td>
<td>Learning to Initialize Generalized Benders Decomposition via Active Learning</td>
<td>Ilias Mitrai (University of Minnesota)</td>
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<tr>
<td>2:25 p.m. to 2:50 p.m.</td>
<td>Optimization-based Approaches for Design of Chemical Process Families using ReLU Surrogates</td>
<td>Georgia Stinchfield (Carnegie Mellon University)</td>
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<tr>
<td>2:50 p.m. to 3:15 p.m.</td>
<td>Safe Deployment of Reinforcement Learning Using Deterministic Optimization of Trained Neural Networks</td>
<td>Calvin Tsay (Imperial College London)</td>
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</tr>
<tr>
<td>3:15 p.m. to 3:40 p.m.</td>
<td>A Gaussian Process Embedded Feature Selection Method Based on Automatic Relevance Determination</td>
<td>Yushi Deng (Auburn University)</td>
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<tr>
<td>3:40 p.m. to 4:10 p.m.</td>
<td>Refreshment Break</td>
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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)
Towards Optimal Energy-water Supply System Operation for Agricultural and Metropolitan Ecosystems
Marcello Di Martino (Texas A&M University)
A Conditional Value-at-Risk Framework for Optimal Microgrid Day-ahead Market Bidding
Robert Herding (University College London)
Stochastic Programming of Energy System Operations Considering Terminal Energy Storage Levels
Teemu Ikonen (Aalto University)
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)
Applied Topology and Geometry in Process Monitoring and Fault Detection
Alexander Smith (University of Minnesota)
Application of Grey-box Modeling for System Health Monitoring in Manufacturing
Utsav Awasthi (University of Connecticut)
Data-based Modeling and Control of Nonlinear Process Systems Using Sparse Identification: An Overview of Recent Results
Panagiotis Christofides (University of California – Los Angeles)
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)

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

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)

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