ADVANCED PSE+ STAKEHOLDER SUMMIT

Pittsburgh Marriott City Center,
Pittsburgh, PA

SEPTEMBER 18–19, 2024

IDAES
Institute for the Design of Advanced Energy Systems

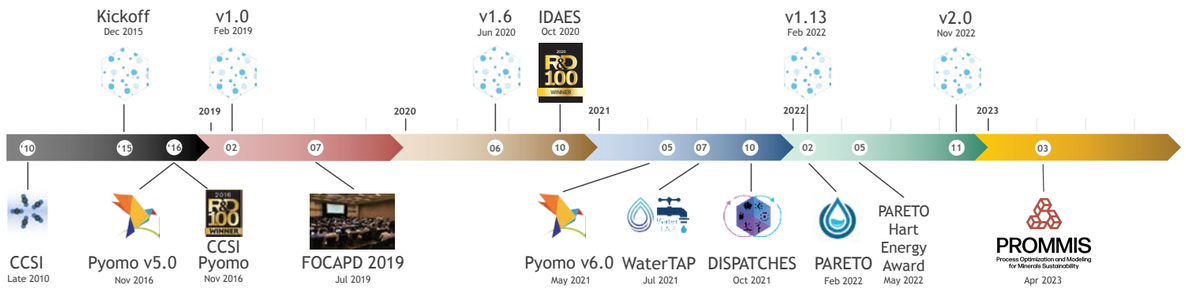
CCSI²
Carbon Capture Simulation for Industry Impact

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

Water TAP

OVERVIEW

A broad set of advanced simulation and optimization tools has changed the landscape around how new process technologies are developed, tested, and demonstrated. These integrated simulation and optimization systems initially developed to support the acceleration and commercialization of carbon capture (CCSI^2) and advanced energy technologies (IDAES) have proven their capability in an ever-widening set of process applications, including water treatment and purification (NAWI WaterTAP) and strategic minerals refining (PROMMIS).



The Advanced Process Systems Engineering (PSE+) Stakeholder Summit provides an annual forum for all parties involved in advanced process development and optimization to have a two-day review of key advances and applications of these new process simulation and optimization capabilities and to join in creating future directions and applications to best utilize these capabilities to accelerate the commercial application of advanced process technology.

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IDAES Institute for the Design of Advanced Energy Systems

CCSI^2 Carbon Capture Simulation for Industry Impact

PROMMIS Process Optimization and Modeling for Minerals Sustainability

WaterTAP

Partner PSE+ Institutions:

National Energy Technology Laboratory

Oak Ridge National Laboratory

Berkeley Lab

Lawrence Livermore National Laboratory

Idaho National Laboratory

Los Alamos National Laboratory

NREL Transforming Energy

Sandia National Laboratories

Pacific Northwest National Laboratory

University of Pittsburgh

West Virginia University

University of Notre Dame

Georgia Tech

The University of Texas at Austin

Carnegie Mellon University

The University of Toledo

WORKSHOP AGENDA

WEDNESDAY – SEPTEMBER 18

7:30	**ARRIVAL AND CONTINENTAL BREAKFAST**	
8:15	**Welcome. Introduction.**	John Shinn (LBNL)
8:30	**CCSI² - Overview, Core Capabilities, and Directions**	Tim Fout (FECM), Mike Matuszewski (NETL)
9:15	**IDAES - Overview, Core Capabilities, and Directions**	Eva Rodezno (FECM), Tony Burgard (NETL), Debangsu Bhattacharyya (WVU)
10:00	**BREAK**	
10:15	**WaterTAP - Overview, Core Capabilities, and Directions**	Kris Villez (ORNL), Tim Bartholomew (NETL)
11:00	**PrOMMiS - Overview, Core Capabilities, and Directions**	Gabby Ubay (FECM), Tom Tarka (NETL), Carl Laird (CMU)
11:45	**Poster Session Preview** Brief descriptions of posters to assist participants in choosing areas of greatest individual relevance.	
12:00	**LUNCH**	
12:45	**Poster Session**	
1:30	**Panel 1 – Hot Topics Introductions**	Steve Burroughs (University of Waikato), Ben Lincoln (University of Waikato), Leslie Miller (OLI), Dan Gunter (LBNL), Rouzbeh Jafari (TCM)
2:30	**Panel 2 – Enabling Future Optimization: Math and Algorithm Research Needs**	Larry Biegler (CMU) Clas Jacobson (Carrier) John Siirola (Sandia)
3:00	**BREAK AND POSTERS**	
3:30	**Timeline and Scope of CCSI2's Involvement in Large-Scale Pilots**	Mike Matuszewski (NETL), Abby Nachtsheim (LANL), Josh Morgan (NETL)
4:00	**Expansion Planning of Reliable and Carbon Neutral Power Systems, San Diego Case Study**	Ben Omell (NETL), Seolhee Cho (CMU), John Siirola (Sandia)
4:30	**Incorporating Detailed Water Chemistry into Process-Scale Cost Optimization with Machine Learning**	Alex Dudchenko (SLAC)
5:00	**Detailed Walkthrough of UKy Flowsheet**	Tom Tarka (NETL), Alejandro Garciadiego (NETL), Andrew Lee (NETL)
5:30	**BREAK AND INFORMAL DISCUSSIONS**	
6:30	**DINNER**	

THURSDAY – SEPTEMBER 19

7:30	**ARRIVAL AND CONTINENTAL BREAKFAST**	
8:15	**The IDAES/PSE+ Software Ecosystem**	Keith Beattie (LBNL)
8:30	**Scaling and Diagnostics**	Andrew Lee (NETL), John Siirola (Sandia)
9:00	**Surrogate Modeling Capabilities**	Carl Laird (CMU), Georgia Stinchfield (CMU)
9:30	**Multi-Period Optimization for Process Design and Market Integration**	Radhakrishna Tumbalam-Gooty (NETL)
10:00	**Dynamic Flowsheeting**	Doug Allan (NETL)
10:30	**BREAK AND POSTERS**	
11:00	**1st-Principles Modeling of Sorbent-Based DAC Systems**	Daison Yancy Caballero (NETL), Ryan Hughes (NETL)
11:30	**IDAES Flowsheet Visualizer; Water & PrOMMiS GUI's; Future Plans; Discussion**	Dan Gunter (LBNL)
12:00	**LUNCH**	
1:00	**Model-based Design of Experiments with Pyomo.DOE**	Alex Dowling (Notre Dame), Dan Laky (Notre Dame)
2:30	**Robust Optimization with PyROS**	Chrysanthos Gounaris (CMU), Jason Sherman (CMU)
3:30	**BREAK AND POSTERS**	
4:00	**AI/ML Approaches to MIPs**	Nick Sahinidis (Georgia Tech)
4:30	**Flexible Environments for Generator and Transmission Expansion Planning (GTEP) Analysis**	Kyle Skolfield (Sandia), John Siirola (Sandia)
5:00	**Directly Integrating Water Chemistry from Reaktoro with Pyomo**	Alex Dudchenko (SLAC)
5:30	**CONCLUSION OF STAKEHOLDER MEETING**	

THURSDAY – SEPTEMBER 19 *(cont.)*

Interactive Discussion of Day 1 Panel Topics Breakout

8:30	**Building an IDAES GUI**	Steve Burroughs (University of Waikato), Ben Lincoln (University of Waikato)
9:30	**PSE User Interfaces Demonstration, Q&A Feedback**	Dan Gunter (LBNL)
10:30	**BREAK AND POSTERS**	
11:00	**Merging IDAES with Commercial Models. Forward Directions.**	Leslie Miller (OLI)
12:00	**LUNCH**	
1:00	**CCSI² Partnership Directions**	Ben Omell (NETL), Mike Matuszewski (NETL), Rouzbeh Jafari (TCM)
2:00	**CONCLUSION OF BREAKOUT SESSION**	

WaterTAP Breakout

8:30	**Enabling High Recovery with Flow Reversal Reverse Osmosis**	Zach Binger (NREL)
8:55	**Assessing Electrodialysis Systems for Concentrating High-Salinity Brines**	Hunter Barber (WVU)
9:25	**Valuing Energy Flexibility in Desalination**	Akshay Rao (Stanford)
9:50	**Bridging Thermodynamic Data and Technoeconomic Assessment for Solvent Extraction**	Alejando Garciadiego (NETL)
10:15	**Water Management R&D at FECM**	Hichem Hadjeres (DOE)
10:30	**CONCLUSION OF BREAKOUT SESSION, BREAK AND POSTERS**	

CCSI² Partnership Dialogues Breakout

8AM–5PM	**Agenda TBD**

PrOMMiS Partnership Opportunities Breakout

8AM–5PM	**Agenda TBD**

POSTERS

Available Day 1 Lunch and Dinner, Day 2 All Day (in program area breakouts)

CCSI²:

- **Jacobian-based Model Diagnostics and Application to Equation Oriented Modeling of a Carbon Capture System** – Douglas Allan (NETL)
- **Model-Based Sequential Design of Experiments for Pilot Testing of Novel Water-Lean CO_2 Capture Solvent** – Anca Ostace (NETL)
- **Optimal Design and Operation of Intensified Towers for CO_2 Capture with Internal, 3-D Printed Heat Exchangers** – Stephen Summits (WVU)
- **Optimal Design and Operation of a Solvent-Sorbent Hybrid CO_2 Capture Process for Minimizing the Cost of High Capture** – Pooja Kasturi (WVU)
- **Robust Design of a Carbon Capture Flowsheet Using PyROS** – Jason Sherman (CMU)
- **Techno-Economic Analysis and Optimization of Point Source Solvent-Based Carbon Capture Systems at High CO_2 Capture Levels for NGCC Power Plants** – Anuja Deshpande (NETL)
- **Validation Framework for Post-Combustion Carbon Capture CFD Simulations** – Grigorios Panagakos (NETL)

Carbon Dioxide Removal:

- **Modeling and Analysis of Climate Variation Effects on Fixed-Bed Direct Air Capture Systems** – Ryan Hughes (NETL)

IDAES:

- **Beyond Price-Taker: Multiscale Optimization of Wind and Battery Integrated Energy Systems** – Xinhe Chen (Notre Dame)
- **IDAES-PSE Software Tools for Optimizing Energy Systems and Market Interactions** – Daniel Laky (Notre Dame)
- **Model Diagnostics for Equation Oriented Models: Roadblocks and the Path Forward** – Andrew Lee (NETL)
- **Efficient Global Optimization for Design of Chemical Process Families** – Ali Asger (CMU), Georgia Stinchfield (CMU)
- **Optimization Model and Solution Strategy for Infrastructure Planning of Reliable and Carbon-Neutral Power Systems: Application to San Diego County** – Seolhee Cho (CMU)
- **Optimal Schedule, Design, and Operation of Solid Oxide Electrolysis Cell Systems Accounting for Long-Term Performance and Health Degradation** – Nishant Giridhar (WWU)

Industry Collaborations:

- **Equation-Oriented Modeling of a Second-Generation Post-Combustion Carbon Capture Process in the IDAES Platform for Economic Optimization** – Ilayda Akkor (CMU)
- **OLI Software: Thermodynamic Modeling Tool for Critical Materials** – Gaurav Das (OLI), Andre Anderko (OLI)

Point Source Capture:

- **Optimization of Membrane-based Carbon Capture using Dimensional Analysis, CFD and Process System Engineering** – Hector Alejandro Pedrozo (CMU)
- **CFD Modeling of High-Flux Plate-and-Frame Membrane modules for Industrial Carbon Capture** – Cheick Dosso (CMU)

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PrOMMiS:

- **Conceptual Design Optimization of Solvent Extraction Processes for REE/CM Recovery** – Norman Tran (CMU)
- **Design and Optimization of Processes for Recovering Rare Earth Elements from End-of-Life Hard Disk Drives** – Chris Laliwala (CMU)
- **Ion Exchange for the Separation of Rare Earth Elements** – Soraya Rawlings (Sandia), Bethany Nicholson (Sandia), John Siirola (Sandia)
- **Opportunities for Process Intensification with Membranes to Promote Circular Economy Development for Critical Minerals** – Molly Dougher (Notre Dame)
- **PrOMMiS Unit Model Library** – Alejandro Garciadiego (NETL)
- **Robust Optimization of Critical Mineral Membrane Separations Under Uncertainty** – Jason Yao (CMU)
- **Steady-State and Dynamic Modeling of a Solvent Extraction Process for Recovery of Rare Earth Elements** – Arkoprabho Dasgupta (WVU)
- **Systematic Design of Complex Processes using GDP: A Comparison of Reformulations** – Emma Johnson (Sandia), Michael Bynum (Sandia), John Siirola (Sandia)

WaterTAP:

- **Bipolar Membrane Electrodialysis in WaterTAP** – Johnson Dhanasekaran (ORNL)
- **Corrosion Informed Costing** – Carson Tucker (Stanford)
- **Cost-optimal Selection of pH Control for Mineral Scaling Prevention in High Recovery Reverse Osmosis Desalination** – Oluwamayowa Amusat (LBNL)
- **Industry Standard Biological Wastewater Treatment in WaterTAP** – Chenyu Wang (NETL), Marcus Holly (NETL)
- **Multi-period Modeling for Solar Thermal Driven Water Treatment** – Mukta Hardikar (NREL)
- **Value of Feed Spacer Optimization in Reverse Osmosis** – Charan Samineni (Stanford)

NOTES

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NOTES

For questions about agenda content and planning, please contact:

Dr. John Shinn, CCSI², IDAES, PrOMMiS Stakeholder Coordinator – *johnhshinn@gmail.com*.

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