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

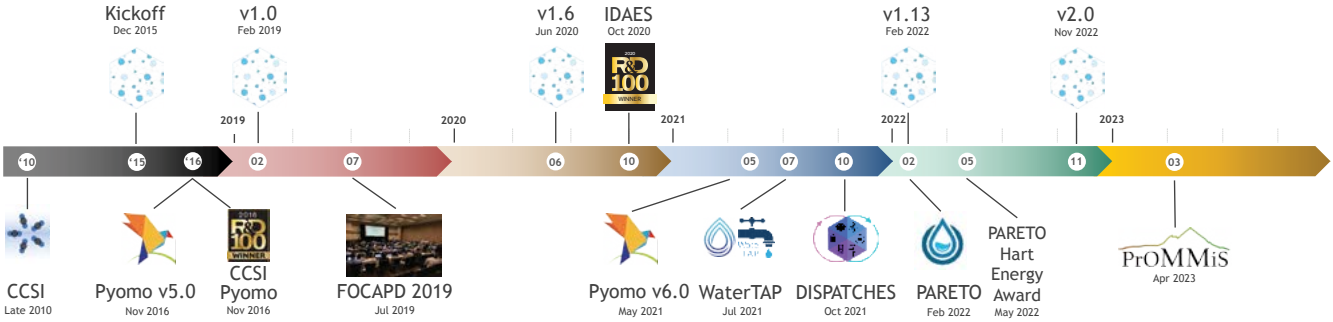
NAWI
National Alliance for Water Innovation

Water TAP

PrOMMiS

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 (CCSI²) 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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Partner PSE+ Institutions:

National Energy Technology Laboratory

Oak Ridge National Laboratory

Berkeley Lab

Lawrence Livermore National Laboratory

INL 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

Texas 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**	Capture Program Leadership TBD (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**	NAWI Leadership TBD, Tim Bartholomew (NETL)
11:00	**PrOMMiS - Overview, Core Capabilities, and Directions**	PrOMMiS - Overview, Core Capabilities, and Directions
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	**Stakeholder Panel Discussion**	John Shinn (LBNL)
2:30	**Timeline and Scope of CCSI2's Involvement in Large-Scale Pilots**	Mike Matuszewski (NETL), Abby Nachtsheim (LANL), Josh Morgan (NETL)
3:00	**1st-Principles Modeling of Sorbent-Based DAC Systems**	Daison YancyCaballero (NETL), Ryan Hughes (NETL)
3:30	BREAK AND POSTERS	
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), Tim Bartholomew (NETL)
5:00	**Detailed Walkthrough of UKy Flowsheet**	Tom Tarka (NETL), Alejandro Garciadiego (NETL), Andrew Lee (NETL)
5:30	BREAK AND INFORMAL CONVERSATIONS	
6:00	DINNER	

THURSDAY – SEPTEMBER 18

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), Oluwamayowa Amusat (LBNL)
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	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)
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	Water Chemistry Using Machine Learning and Reaktoro	Alex Dudchenko (SLAC), Savannah Sakhai (WVU), Ilayda Akkor (CMU)
5:30	CONCLUSION OF STAKEHOLDER MEETING	

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)
- **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)
- **Recent Advances of PyROS: A Pyomo Solver for Nonconvex Two-Stage Robust Optimization in Process Systems Engineering** – Jason Sherman (CMU)

DISPATCHES:

- **Conceptual Design of Integrated Energy Systems with Market Interaction Surrogate Models** – Xinhe Chen (Notre Dame)

DOW

- **Equation-Oriented Modeling of a Second-Generation Post-Combustion Carbon Capture Process in the IDAES Platform for Economic Optimization** – Ilayda Akkor (CMU)

IDAES:

- **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)
- **Optimal Design Approaches for Cost-Effective Manufacturing and Deployment of Chemical Process Families with Economies of Numbers** – Georgia Stinchfield (CMU)
- **Optimal Schedule, Design, and Operation of Solid Oxide Electrolysis Cell Systems Accounting for Long-Term Performance and Health Degradation** – Nishant Giridhar (WWU)

PrOMMiS:

- **Design and Optimization of Processes for Recovering Rare Earth Elements from End-of-Life Hard Disk Drives** – Chris Laliwala (CMU)
- **Optimizing Batch Crystallization with Model-based Design of Experiments** – Hailey Lynch (Notre Dame)
- **Opportunities for Process Intensification with Membranes to Promote Circular Economy Development for Critical Minerals** – Molly Dougher (Notre Dame)
- **Optimal Membrane Cascade Design for Critical Mineral Recovery Through Logic-based Superstructure Optimization** – Daniel Ovalle (CMU)
- **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)

WaterTAP:

- **Incorporating Detailed Water Chemistry with Surrogate Models** – Oluwamayowa Amusat (LBNL)
- **Modeling Industry Standard Biological Wastewater Treatment** – Chenyu Wang (NETL), Marcus Holly (NETL)
- **WaterTAP Model Library** – Adam Atia (NETL)
- **Representing Processes Over Time with Multiperiod Modeling** – Zachary Binger (NREL), Mukta Hardikar (NREL)

For questions about agenda content and planning, please contact:

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