ADVANCED PSE+ STAKEHOLDER SUMMIT

The Westin Pittsburgh,
Pittsburgh, PA

SEPTEMBER 3–4, 2025

IDAES
Institute for the Design of Advanced Energy Systems

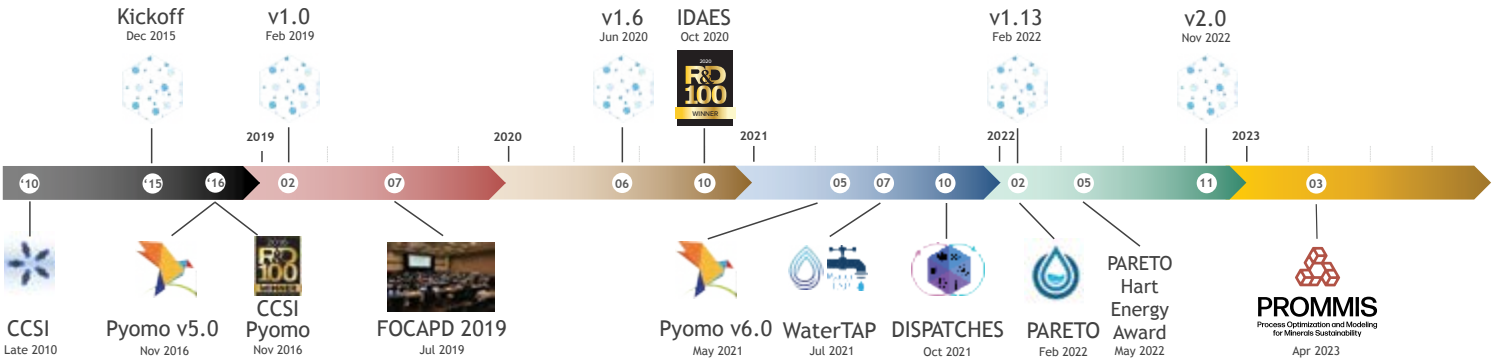
CCSI²
Carbon Capture Simulation for Industry Impact

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

Water TAP

OVERVIEW

The continued development and growing adoption of advanced simulation and optimization capabilities are driving a significant evolution in process technology innovation. Initially developed to accelerate the design and deployment of carbon capture technologies and advanced energy systems, the Carbon Capture Simulation Initiative (CCSI) toolset and Institute for the Design of Advanced Energy Systems (IDAES) Integrated Platform have now demonstrated broad utility across an expanding range of applications, including water treatment and purification (WaterTAP) and strategic minerals refining (PrOMMiS). Collectively, these sophisticated digital platforms, now referred to as the IDAES+ ecosystem, provide a powerful framework for accelerating innovation by enabling rapid prototyping, rigorous performance prediction, and comprehensive economic evaluation of new technologies, ultimately mitigating risks and reducing the time and cost associated with translating laboratory discoveries into commercial realities across these vital sectors.



The annual Advanced Process Systems Engineering (PSE+) Stakeholder Summit is a two-day forum convening stakeholders from across academia, industry, and government. It provides a comprehensive review of recent advances and novel applications, while facilitating collaborative discussions aimed at broadening the adoption of advanced process systems engineering capabilities.

Please join us in shaping the future of Process Systems Engineering!

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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

The University of Texas at Austin

Carnegie Mellon University

The University of Toledo

WORKSHOP AGENDA

WEDNESDAY – SEPTEMBER 3

7:30	**ARRIVAL AND CONTINENTAL BREAKFAST**	
8:15	**Welcome, Introduction**	John Shinn (LBNL)
8:30	**Carbon Capture Simulation for Industry Impact**	Tim Fout (FECM), Mike Matuszewski (NETL)
9:05	**IDAES – Core Overview, Core Capabilities, Directions**	Eva Rodezno (FECM), Tony Burgard (NETL)
9:40	**Process Optimization and Modeling for Minerals Sustainability (PrOMMiS)**	Gabby Ubay (FECM), Tom Tarka (NETL)
10:15	**BREAK**	
10:35	**Water treatment Technoeconomic Assessment Platform (WaterTAP)**	Adam Atia (NETL)
11:10	**Common Software Development and Release Process**	Keith Beattie (LBNL)
11:45	**Poster Session Preview** Brief descriptions of posters to assist participants in choosing areas of greatest individual relevance.	Miguel Zamarripa (NETL)
12:00	**LUNCH**	
12:45	**Poster Session**	
1:30	**Panel Discussion: Supporting the Future of PSE**	
2:30	**Sequential Design of Experiments (SDoE) Framework to Maximize the Value of Experimental Data**	Abby Nachtsheim (LANL)
2:55	**eNMPC & Additional Insights**	Larry Biegler (CMU)
3:20	**Generalized Generation & Transmission Expansion Planning using IDAES-GTEP**	Ben Omell (NETL), Kyle Skolfield (Sandia)
3:45	**BREAK AND POSTERS**	
4:15	**Project Ahuora, Capabilities, Directions**	Tim Walmsley (U of Waikato)
4:40	**PRIMA & PRIMO Overview & Live Demo**	Markus Drouven (NETL)
5:05	**PARETO & AquaTrade Overview & Live Demo**	Philip Tominac (NETL)
5:30	**BREAK AND INFORMAL DISCUSSIONS**	
6:00	**DINNER**	

THURSDAY – SEPTEMBER 4

7:30	**ARRIVAL AND CONTINENTAL BREAKFAST**	
8:00	**IDAES+ Software Ecosystem**	Keith Beattie (LBNL)
	New Documentation and Organization	Ludovico Bianchi (LBNL)
	Tutorial and Training Updates	Miguel Zamarripa (NETL)
	Pyomo Advances	John Siirola (Sandia)
	Facilitating Model Building/Convergence	Alejandro Garciadiego (NETL), John Siirola (Sandia)
	Flowsheet Visualization and Graphical User Interfaces	Dan Gunter (LBNL)
9:30	**BREAK AND POSTERS**	
	Advanced PSE Tools	
10:00	**Conceptual Design**	Carl Laird (CMU)
10:20	**Surrogate Modeling**	Oluwamayowa Amusat (LBNL)
10:40	**Leveraging AI/ML**	Nick Sahinidis (Georgia Tech)
11:00	**Robust Optimization**	Jason Sherman (CMU)
11:20	**Design of Experiments**	Alex Dowling (ND)
11:40	**Dynamic Optimization**	Nishant Giridhar (WVU), Debangsu Bhattacharyya (WVU)
12:00	**LUNCH**	
1:00	**WaterTAP Demos**	Marcus Holly (NETL)
1:45	**PrOMMiS Flowsheet Construction**	Marcus Holly (NETL)
2:30	**BREAK**	
3:00	**Costing Examples – Basic**	Brandon Paul (NETL)
3:45	**Costing Examples – Advanced Features**	Brandon Paul (NETL)
4:45	**CONCLUDING REMARKS**	

THURSDAY – SEPTEMBER 4 *(cont.)*

Breakout Room #1

8:00	**CCSI² Framework for Framework for Optimization, Quantification of Uncertainty and Surrogates (FOQUS) Demo**	Katherine Hedrick (NETL), Anuja Deshpande (NETL)
9:30	**BREAK AND POSTERS**	
10:00	**IDAES Basics Demo**	Doug Allan (NETL), Will Strahl (NETL)
12:00	**LUNCH**	
1:00	**Ad-Hoc Discussions**	
2:30	**BREAK**	
3:00	**Ad-Hoc Discussions**	

Breakout Room #2

8:00	**WaterTAP Discussions**	Adam Atia (NETL)
9:30	**BREAK AND POSTERS**	
10:00	**WaterTAP Discussions**	Adam Atia (NETL)
12:00	**LUNCH**	
1:00	**Project Ahuora Discussions**	Tim Walmsley (U. of Waikato)
2:30	**BREAK**	
3:00	**Project Ahuora Discussions**	Tim Walmsley (U. of Waikato)

Breakout Room #3

8:00	**CCSI² Discussions**	Mike Matuszewski (NETL), Ben Omell (NETL)
9:30	**BREAK AND POSTERS**	
10:00	**CCSI² Discussions**	Mike Matuszewski (NETL), Ben Omell (NETL)
12:00	**LUNCH**	
1:00	**PrOMMiS Discussions**	Tom Tarka (NETL), Alison Fritz (NETL)
2:30	**BREAK**	
3:00	**PrOMMiS Discussions**	Tom Tarka (NETL), Alison Fritz (NETL)

POSTERS

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

CCSI²:

- **FOQUS Updates and Development Process** – Keith Beattie (LBNL)
- **Pilot Support: EEMPA Solvent Interfacial Area Modeling** – Jay Xu (PNNL)
- **Pilot Support: GTI Dynamic Rotating Packed Bed Contactor Modeling** – Jay Xu (PNNL)
- **Accelerating CO_2 Capture Process Design with Machine Learning-based Surrogates** – Phan Nguyen (LLNL)
- **Process Optimization of Absorption System with Topological Optimization of Intensified Structured Packing** – Debangsu Bhattacharyya (WVU)
- **Process Modeling and Techno-Economic Optimization Using Hybrid Solvent-Sorbent Post-Combustion Capture** – Debangsu Bhattacharyya (WVU)
- **Pilot Support: Process Modeling and Optimization of Post Combustion Capture Technology for Nucor Steel Production** – Anuja Deshpande (NETL)
- **Pilot Support: SDOE for MTR Membrane Technology Testing at Wyoming Integrated Test Center** – Daison Caballero (NETL)
- **Broad Range Capture and Uncertainty Quantification** – Lingyan Deng (NETL)
- **Robust Optimization of MEA Solvent Process** – Jason Sherman (CMU)
- **PyROS Robust Optimization Tool Overview** – Chrysanthos Gounaris (CMU)
- **Pilot Support: Membrane Based CO_2 Capture Process at US Steel and SDoE Support** – Glenn Lipscomb (Toledo)
- **Pitfalls and Successes of High-Fidelity Modeling for Piperazine** – Gary Rochelle (Texas at Austin)
- **Uncertainty Quantification and Sensitivity Analysis in CO_2 Removal Models Using Pyomo.DoE** – Shuvashish Mondal (Notre Dame), Alex Dowling (Notre Dame)
- **Membrane Modeling Framework for Industrial Carbon Capture** – Katherine Hedrick (NETL)

IDAES:

- **Efficient Design and Deployment of Process Families using IDAES Models** – Ali Asger (CMU)
- **Impact of Carbon Capture Requirements and Flexibility Attributes on NGCC Plant Profitability: A Combined Process and Market Dispatch Analysis** – Radhakrishna Tumbalam-Gooty (NETL)
- **Integrated Technology for Cost-Effective CO_2 Capture and Formic Acid Production: Modeling, Optimization, and Economic Analysis** – Maojian Wang (NETL)
- **The Economic Benefit of Dynamic Generation: Assessing the Value of a Fast-Response Power Plant** – Jinliang Ma (NETL)
- **Harnessing SOFC-SOEC Flexibility: Minimizing the System Scale for Economic Viability Across Diverse Market Scenarios** – Ruonan Li (NETL)
- **Optimal Design of Liquid Oxygen Storage System for Flexible Operation of a Direct-Fired Supercritical CO_2 Power Cycle** – Radhakrishna Tumbalam-Gooty (NETL)
- **An Improved Price-taker Approach for the Optimization of Integrated Energy Systems** – Xinhe Chen (Notre Dame), Kay Lu (Notre Dame), Alex Dowling (Notre Dame)
- **Expanding Optimal Experimental Design using Grey Box Design Criteria in Pyomo. DoE** – Dan Laky (Notre Dame), Alex Dowling (Notre Dame)

PrOMMiS:

- **Conceptual Design Strategies for Solvent Extraction Trains** – (preliminary) Norman Tran (CMU), Carl Laird (CMU)
- **Steady-State and Dynamic Modeling of Conventional and Membrane Solvent Extraction Units** – (preliminary) Arkoprabho Dasgupta (WVU), Doug Allan (NETL), Alejandro Garciadiego (NETL), Marcus Holly (NETL), Debangsu Bhattacharyya (WVU)
- **Steady-State and Dynamic Modeling of Leaching Units** – (preliminary) Akintomiwa Ojo (WVU), Arkoprabho Dasgupta (WVU), Alejandro Garciadiego (NETL), Marcus Holly (NETL), Debangsu Bhattacharyya (WVU)
- **Steady-State Modeling of Rare Earth Element Extraction and Separation** – (preliminary) Marcus Holly (NETL), Alejandro Garciadiego (NETL), Doug Allan (NETL), Arkoprabho Dasgupta (WVU)
- **Data-driven modeling and optimization of critical minerals processes** – (preliminary) Dimitris Farids (Georgia Tech), Nick Sahinidis (Georgia Tech)
- **Robust Membrane Process Design for Recovery of Critical Minerals Under Uncertainty** – (preliminary) Jason Yao (CMU), Chrysanthos Gounaris (CMU)
- **Ion Exchange for the Separation of Rare Earth Elements** – (preliminary) Authors: Edna Soraya Rawlings (Sandia), Bethany Nicholson (Sandia), John Siirola (Sandia)
- **Science-Based Design of Experiments to Facilitate the Scale-Up of Novel Critical Minerals and Materials Separation** – Shammah Lilonfe (Notre Dame), Alex Dowling (Notre Dame)
- **A Multi-Component Membrane Model to Enable Design and Scale-Up of Multi-Stage Diafiltration Cascades for Critical Mineral Recovery** – Molly Dougher (Notre Dame), Alex Dowling (Notre Dame)
- **1Flowsheet Optimization for Critical Minerals** – Michael Bynum (Sandia), Marcus Holly (NETL), Alejandro Garciadiego (NETL), Brandon Paul (NETL), Edna Soraya Rawlings (Sandia), Bethany Nicholson (Sandia)
- **1Design and Optimization of Processes for Recovering Rare Earth Elements from End-of-Life Permanent Magnets** – (preliminary) Chris Laliwala (CMU), Oluwamayowa O. Amusat (LBNL), Ana I. Torres (CMU)

Produced Water Partnership

- **Optimization of Strategic and Operational Decisions for the Recovery of Critical Minerals from Produced Water Networks** – Arsh Bhatia (CMU)

WaterTAP:

- **Overview of Water treatment Technoeconomic Assessment Platform: WaterTAP** – Kurban Sitterley (NREL), Elmira Shamlou (NETL), Chenyu Wang (NETL), Adam A. Atia (NETL)
- **Biological Wastewater Treatment and Resource Recovery in WaterTAP** – Chenyu Wang (NETL), Maojian Wang (NETL), Marcus Holly (NETL), Alejandro Garciadiego (NETL), Adam A. Atia (NETL)
- **Flexible Desalination to Increase Resiliency of Energy-Water Infrastructure** – Akshay Rao (Stanford), Radhakrishna Tumbalam-Gooty (NETL), Marcus Holly (NETL), Mukta Hardikar (NREL), Kurban Sitterley (NREL), Adam A. Atia (NETL)
- **Integrating Detailed Chemistry with Process Modeling in WaterTAP** – Carson Tucker (Stanford), Savannah Sakhai (WVU), Oluwamayowa Amusat (LBNL), Zhuoran Zhang (Columbia U), Alexander Dudchenko (SLAC), Adam A. Atia (NETL)
- **The Future of WaterTAP: Pathways to Industry Adoption and a Call to Action** – Elmira Shamlou (NETL), Daniel Gunter (LBNL), Keith Beattie (LBNL), Mukta Hardikar (NREL), Kurban Sitterley (NREL), Adam A. Atia (NETL)

NOTES

For questions about agenda content and planning, please contact:

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