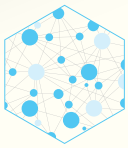
ADVANCED PSE+ STAKEHOLDER SUMMIT

The Westin Pittsburgh,
Pittsburgh, PA

SEPTEMBER 3–4, 2025



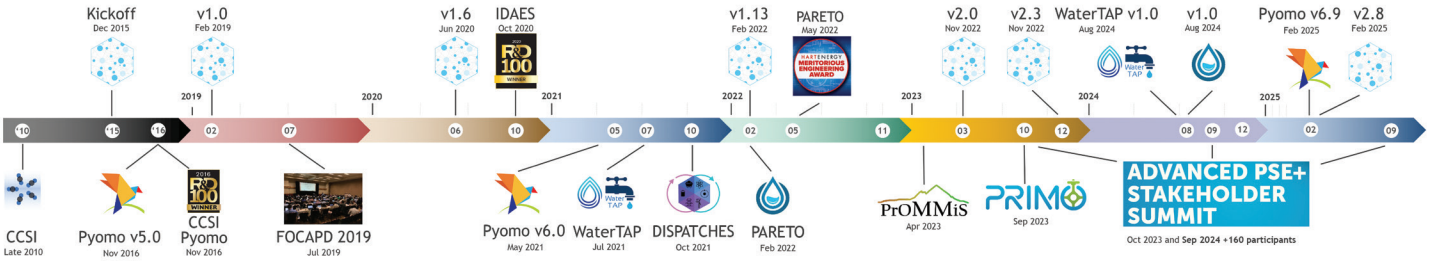
IDAES
Institute for the Design of Advanced Energy Systems

CCSI^2
Carbon Capture Simulation for Industry Impact

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

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 Technoeconomic Assessment Platform (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!

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

Partner PSE+ Institutions:

NETL 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)
8:45	**IDAES – Core Overview, Core Capabilities, Directions**	Eva Rodezno (FECM), Tony Burgard (NETL)
9:15	**Carbon Capture Simulation for Industry Impact (CCSI²)**	Mike Matuszewski (NETL)
9:45	**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), Mike Matuszewski (NETL), Alex Dowling (ND)
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**	
	Main Room	
8:00	**IDAES+ Software Ecosystem**	Keith Beattie (LBNL)
8:00	**New Documentation and Organization**	Ludovico Bianchi (LBNL)
8:15	**Tutorial and Training Updates**	Miguel Zamarripa (NETL)
8:30	**Pyomo Advances**	John Siirola (Sandia)
8:50	**Facilitating Model Building/Convergence**	Alejandro Garciadiego (NETL), John Siirola (Sandia)
9:10	**User Interfaces for IDAES+ Projects**	Sarah Poon (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 Demo**	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 Optimization, Quantification of Uncertainty and Surrogates (FOQUS) Demo**	Anuja Deshpande (NETL)
9:30	**BREAK AND POSTERS**	
10:00	**IDAES Basics Demo**	Will Strahl (NETL), Douglas Allan (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 EEMPA SDOE & Modeling**	Josh Morgan (NETL), Abby Nachtsheim (LANL)
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:

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

IDAES:

1. **An Improved Price-taker Approach for the Optimization of Integrated Energy Systems** – Xinhe Chen (Notre Dame), Daniel Laky (Notre Dame), Kay Lu (Notre Dame), Alex Dowling (Notre Dame)

2. **Efficient Design and Deployment of Process Families using IDAES Models** – Ali Asger (CMU)

3. **Harnessing SOFC-SOEC Flexibility: Minimizing the System Scale for Economic Viability Across Diverse Market Scenarios** – Ruonan Li (NETL), Alexander Noring (NETL)

4. **IDAES Flowsheet of CO_2 to Methanol Conversion Process** – Dev Kakkad (NETL), Maojian Wang (NETL), Daison Caballero (NETL), Miguel Zamarripa (NETL), Joshua Morgan (NETL)

5. **Impact of Carbon Capture Requirements and Flexibility Attributes on NGCC Plant Profitability: A Combined Process and Market Dispatch Analysis** – Radhakrishna Tumbalam-Gooty (NETL)

6. **Integrated Technology for Cost-Effective CO_2 Capture and Formic Acid Production: Modeling, Optimization, and Economic Analysis** – Maojian Wang (NETL)

PrOMMiS:

1. **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)

2. **An Optimization-Based Law of Mass Action Precipitation/Dissolution Model** – Chris Laliwala (CMU), Oluwamayowa O. Amusat (LBNL), Ana I. Torres (CMU)

3. **Conceptual Design Strategies for Solvent Extraction Trains** – Norman Tran (CMU), Carl Laird (CMU)

4. **Data-Driven Modeling and Optimization of Critical Minerals Processes** – Dimitrios Fardis (Georgia Tech), Nick Sahinidis (Georgia Tech)

5. **Flowsheet Optimization for Critical Minerals** – Michael Bynum (Sandia), Marcus Holly (NETL), Alejandro Garciadiego (NETL), Brandon Paul (NETL), Edna Soraya Rawlings (Sandia), Bethany Nicholson (Sandia)

6. **Ion Exchange for the Separation of Rare Earth Elements** – Edna Soraya Rawlings (Sandia), Bethany Nicholson (Sandia), Ward Burgess (NETL), Charlotte Rutnik (NETL), Nicholas Siefert (NETL), John Siirola (Sandia), John Siirola (Sandia)

7. **New Capabilities in ParmEst and Pyomo.DoE** – Daniel Laky (Notre Dame), Alex Dowling (Notre Dame)

8. **Robust Membrane Process Design for Recovery of Critical Minerals Under Uncertainty** – Jason Yao (CMU), Chrysanthos Gounaris (CMU)

9. **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)

10. **Steady-State and Dynamic Modeling of Conventional and Membrane Solvent Extraction Units** – Arkoprabho Dasgupta (WVU), Douglas Allan (NETL), Alejandro Garciadiego (NETL), Marcus Holly (NETL), Debangsu Bhattacharyya (WVU)

11. **Steady-State and Dynamic Modeling of Leaching Units** – Akintomiwa Ojo (WVU), Arkoprabho Dasgupta (WVU), Alejandro Garciadiego (NETL), Marcus Holly (NETL), Debangsu Bhattacharyya (WVU)

12. **Steady-State Modeling of Rare Earth Element Extraction and Separation** – Marcus Holly (NETL), Alejandro Garciadiego (NETL), Douglas Allan (NETL), Arkoprabho Dasgupta (WVU)

13. **Towards Reliable Optimization of Critical Minerals Process Models** – Michael Bynum (Sandia), Marcus Holly (NETL), Alejandro Garciadiego (NETL), Brandon Paul (NETL), Edna Soraya Rawlings (Sandia), Bethany Nicholson (Sandia)

Produced Water Partnership

1. **Optimization of Strategic and Operational Decisions for the Recovery of Critical Minerals from Produced Water Networks** – Norman Tran (CMU), Arsh Bhatia (CMU), Carl Laird (CMU), Miguel Zamarripa (NETL), Markus Drouven (NETL)

WaterTAP:

1. **Biological Wastewater Treatment and Resource Recovery in WaterTAP** – Chenyu Wang (NETL), Maojian Wang (NETL), Marcus Holly (NETL), Alejandro Garciadiego (NETL), Adam A. Atia (NETL)

2. **Flexible Desalination to Increase Resiliency of Energy-Water Infrastructure** – Akshay K. Rao (Stanford), Radhakrishna Tumbalam-Gooty (NETL), Marcus Holly (NETL), Mukta Hardikar (NREL), Kurban A. Sitterley (NREL), Alexander Dudchenko (SLAC), Adam A. Atia (NETL)

3. **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)

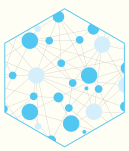
4. **Overview of Water treatment Technoeconomic Assessment Platform: WaterTAP** – Kurban A. Sitterley (NREL), Elmira Shamlou (NETL), Chenyu Wang (NETL), Adam A. Atia (NETL)

5. **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 A. Sitterley (NREL), Adam A. Atia (NETL)

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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