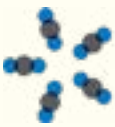
ADVANCED PSE+ STAKEHOLDER SUMMIT I

Westin Hotel and Conference Center,
Tysons Corner, VA

OCTOBER 11–12, 2023

IDAES
Institute for the Design of Advanced Energy Systems



CCSI²
Carbon Capture Simulation for Industry Impact

PrOMMiS

NAWI
National Alliance for Water Innovation

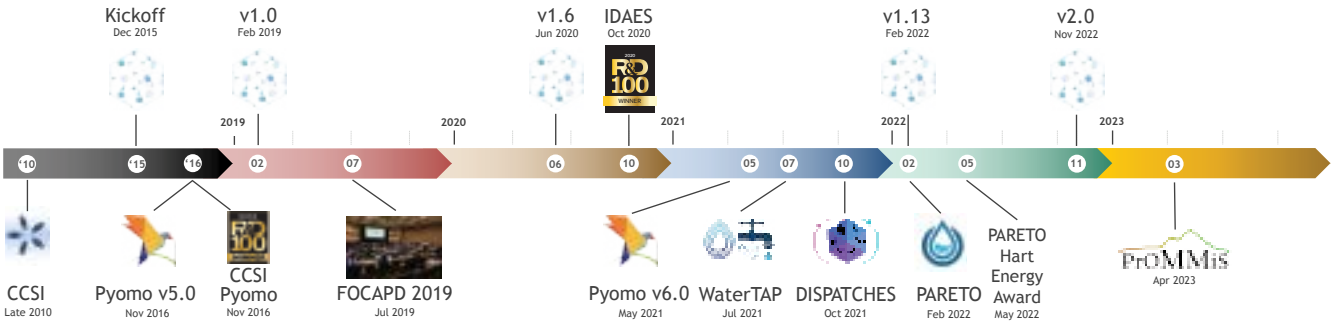
Water TAP

PARETO
The Produced Water Optimization Initiative

DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

OVERVIEW

Since 2010 the Department of Energy in collaboration with the National Energy Technology Laboratory and multiple national laboratories and university partners have maintained a long-range program aimed at developing and utilizing the most advanced algorithms and computational capabilities to dramatically improve the abilities of multi-scale process modeling and optimization for accelerating technology development and reducing technical risk.



Starting from an initial focus on carbon capture technologies and maximizing the capability of existing process simulation platforms (the Carbon Capture Simulation Initiatives, CCSI and CCSI^2), the capabilities have further improved by expanding to advanced multi-scale, integrated energy system applications by developing an entirely new simulation and optimization platform based on the most advanced approaches (the Institute for Design of Advanced Energy Systems – IDAES).

The recognition of the power of these advanced process systems engineering approaches led to additional programs in water treatment (WaterTAP), produced water management (PARETO), and rare earth and critical minerals processing (Process Optimization and Modeling for Minerals Sustainability – PrOMMiS).

Each program grew in partnership with each other and with a full cadre of industrial stakeholders who guided program directions, tested, and improved the tools and capabilities, and generated new high value applications for these advanced capabilities.

This Summit is the first time all of these programs have come together with all of their stakeholders to:

- review in a comprehensive manner what new capabilities have been developed,
- discuss future directions, and
- examine how value is being created in multiple process systems applications.

IDAES
Institute for the Design of Advanced Energy Systems

CCSI²
Carbon Capture Simulation for Industry Impact

DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

NAWI
National Alliance for Water Innovation

Water TAP

PrOMMiS

PARETO
The Produced Water Optimization Initiative

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

WestVirginiaUniversity.

UNIVERSITY OF NOTRE DAME

Georgia Tech

TEXAS The University of Texas at Austin

Carnegie Mellon University

THE UNIVERSITY OF TOLEDO

WORKSHOP AGENDA

WEDNESDAY – OCTOBER 11

7:30	**REGISTRATION, COFFEE AND CONTINENTAL BREAKFAST**	
8:00	**Welcome. Introduction.**	John Shinn, Stakeholder Engagement Lead for IDAES, CCSI², PrOMMiS
8:15	**History and Evolution of Advanced PSE+ Programs**	David Miller, NETL
8:50	**Core PSE+ Programs – Key Capabilities and Directions**	
	Carbon Capture Simulation for Industry Impact (CCSI²)	Michael Matuszewski, Ben Omell, NETL
	Institute for Design of Advanced Energy Systems (IDAES)	Tony Burgard, NETL; Carl Laird, Carnegie Mellon University
10:10	**BREAK AND INFORMAL CONVERSATIONS**	
10:30	**Process-Focused PSE+ Programs**	
	Water treatment Technology Assessment Platform (WaterTAP)	Tim Bartholomew, NETL
	Process Optimization and Modeling for Minerals Sustainability (PrOMMiS)	Thomas Tarka, NETL
	Produced Water Management (PARETO)	Markus Drouven, NETL
	National Emissions Reduction Initiative (NEMRI)	Markus Drouven, NETL
12:00	**Poster Session Preview** Brief descriptions of posters to assist participants in choosing areas of greatest individual relevance.	

12:15 **FULL PSE+ PROGRAM LUNCH AND POSTER SESSION**

1:30 **Applications of Advanced PSE+ Approaches to Accelerate Technology Development and Deployment**

Accelerating Carbon Capture Technology Development in Partnership with CCSI^2	Marty Lail, Research Triangle Institute
Advancing the State of the Art in Expansion Planning for the California Grid in Partnership with IDAES	Chris McLean, California Energy Commission; Ben Omell, NETL; Seolhee Cho, Carnegie Mellon University
Advances in Modeling Power Generation Grid and Market Interactions (DISPATCHES)	Alex Dowling, University of Notre Dame; John Siirola, Sandia National Laboratories
Evaluating Advanced Hybrid Energy Systems with IDAES	Miguel Zamarripa, Daison Caballero, Radhakrishna Tumbalam Gooty, NETL
Incorporating Detailed Water Chemistry with Process-Scale Cost Optimization	Tim Bartholomew, NETL; Leslie Miller, OLI Systems

4:00 **BREAK AND INFORMAL CONVERSATIONS**

4:30 **Stakeholder Panel Discussion**

Stakeholder perspectives on value of Advanced PSE Capabilities and opportunities for further development and applications.

5:30 **CONCLUSION OF AFTERNOON SESSION**

6:00 **DINNER AND POSTER SESSION**

THURSDAY – OCTOBER 12

8:30 **REGISTRATION, COFFEE, CONTINENTAL BREAKFAST AND INFORMAL DISCUSSIONS**

9:00 **Reflections on Day 1. Additional Stakeholder Input.** John Shinn, LBNL

THURSDAY – OCTOBER 12 *(cont.)*

General Session

(to be run in parallel to two project-specific breakout sessions & several ad-hoc tag-ups between technical team members and stakeholders)

9:15	**IDAES for Advanced Users**	
	Model, Flowsheet, and Costing Libraries	Alejandro Garciadiego, NETL
	Making Models Dynamic and Controllable	Doug Allan, NETL
	Tools and Workflows for Surrogate Modeling	Miguel Zamarripa, NETL
	New and Upcoming IDAES Features	
	Diagnostics and Scaling	Andrew Lee, NETL
	Visualization	Dan Gunter, LBNL
11:30	**WaterTAP's Graphical User Interface**	Dan Gunter, Michael Pesce, LBNL
12:00	**FULL PSE+ PROGRAM LUNCH AND POSTER SESSION**	
1:15	**CCSI² for Advanced Users**	
	Design of Experiments	Abby Nachtsheim, LANL; Alex Dowling, University of Notre Dame
	FOQUS Demonstration (Turbine, Sinter, UQ, DOE, Surrogates)	Ryan Hughes, NETL
3:15	**BREAK AND INFORMAL CONVERSATIONS**	
3:30	**PARETO Demonstration**	Markus Drouven, NETL
	Hydraulics Module	Naresh Susarla, NETL
	Rare Earth Element/CM Screening Tool	Carl Laird, Carnegie Mellon University
4:30	**CONCLUSION OF STAKEHOLDER MEETING**	

THURSDAY – OCTOBER 12 *(cont.)*

CCSI² and IDAES Breakout

9:15	**CCSI² Active Collaborations**	
	EPRI – EEMPA Solvent Pilot	Josh Morgan, NETL
	RTI – Gen 2 Non-Aqueous Solvent	Josh Morgan, NETL
	UKy/Nucor – Solvent EAF Pilot	Daison Caballero, NETL
	UT Austin/Honeywell UOP – Piperazine	Gary Rochelle, University of Texas at Austin
	Baxter/Chart – General Cement Cryogenic Capture	Daison Caballero, NETL
	U.S. Steel – Steel Pilot Support	Glenn Lipscomb, University of Toledo
12:15	**FULL PSE+ PROGRAM LUNCH AND POSTER SESSION**	
1:15	**IDAES for Beginners (install, setup, github, etc.)**	Alejandro Garciadiego, NETL
	IDAES Active Collaborations	
	California Energy Commission, Expansion Planning	Ben Omell, NETL
	EMRE – High Capture	Daison Caballero, NETL
	Carrier – Process Family Design	John Siirola, Sandia National Laboratories
	Additional Stakeholder Tag-ups	
	IDAES	John Shinn, NETL
	DISPATCHES	Alex Dowling, University of Notre Dame; John Siirola, Sandia National Laboratories
4:30	**CONCLUSION OF STAKEHOLDER MEETING**	

THURSDAY – OCTOBER 12 *(cont.)*

WaterTAP Breakout

9:15	**Assessing the Cost of GAC and IX Technologies for Treating PFAS**	Hunter Barber, WVU
	Analyzing Solar Driven Desalination Systems	Kurby Sitterley, NREL
	Using Benchmark Simulation Models to Evaluate Biological Wastewater Treatment	Adam Atia, NETL
	WaterTAP Demos	
	Incorporating OLI Calculations	Paul Vecchiarelli, NREL
	Using Parameter Sweep and Analysis Tools	Kinshuk Panda, NREL
	Connecting Flowsheets to the WaterTAP GUI	Michael Pesce, LBNL
12:00	**FULL PSE+ PROGRAM LUNCH AND POSTER SESSION**	
1:15	**Scale Management and Mitigation Utilizing a Novel Theoretical Tool**	Gaurav Das, OLI Systems
	Evaluating Chemical Softening and Electrocoagulation for Brine Pretreatment	Abdiel Lugo, New Mexico State University
	WaterTAP Demos	
	Using Multi-period Modeling	Zach Binger, NREL; Mukta Hardikar, NREL
	Conducting a Parameter Estimation	Savannah Sakhai, West Virginia University
	Incorporating Custom Process and Cost Modeling	Alexander Dudchenko, SLAC
	Evaluating the Design & Operation of an Electrodialysis Desalination System	Xiangyu Bi, LBNL
	Investigating High Pressure Reverse Osmosis	Alexander Dudchenko, SLAC
4:30	**CONCLUSION OF STAKEHOLDER MEETING**	

POSTERS

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

Carbon Dioxide Removal:

- **Process Modeling and Analysis of a Novel Sorbent Material for Direct Air Capture Applications** – Daison Caballero
- **An Optimization Framework for Net Negative NGCC Power Plants** – Alex Noring

General:

- **Open-Source Scientific Software: Community Engagement and Commercial Adoption** – Keith Beattie, Dan Gunter, Ludovico Bianchi

CCSI²:

- **Advanced Solvent Configurations for Superstructure Optimization** – Katherine Hedrick
- **CCSI² Computational Support for Modeling of RTI Non-Aqueous Solvent Technology** – Josh Morgan
- **CFD Simulations for Post-Combustion Carbon Capture** – Grigorios Panagakos
- **Characterizing the Pareto Trade-off between Science-based Information Content and Measurements Cost** – Jialu Wang
- **Designing an Amine-Based CO_2 Absorption System in Light of Epistemic Uncertainty** – Jason Sherman
- **Modeling and Optimization of a Rotary Packed Bed Contactor for CO_2 Capture** – Ryan Hughes
- **Optimization of Intensified Towers with Internal Heat Exchangers for CO_2 Capture** – Stephen Summits
- **Process Intensification: Experimental Scale-up, Solvent & Packing Optimization for Point Source Capture of CO_2** – Costas Tsouris
- **Solvent/packing Interaction & Multiscale Modeling for Pilot Support of Water-lean EEMPA Solvent** – Jay Xu
- **Technical Risk Reduction: Sequential Design of Experiments and Uncertainty Quantification** – Abby Nachtsheim
- **Techno-Economic Analysis and Optimization of NGCC Solvent-based Carbon Capture Systems at High Capture Levels** – Ben Omell

DISPATCHES:

- **Multiscale Optimization of Integrated Energy Systems that Co-Produce Electricity and Hydrogen Using Market Surrogates** – Xinhe Chen, Radhakrishna Tumbalam Gooty
- **Simultaneous Design and Operation of a Fossil-based Hybrid Energy System with Integrated Thermal Energy Storage** – Soraya Rawling, Naresh Susarla

IDAES:

- **Flexible Modular Formulations for Grid Infrastructure Expansion Planning** – Kyle Skolfield
- **IDAES Diagnostics Toolbox** – Andrew Lee
- **IDAES Visualization and User Interfaces** – Dan Gunter
- **ML-Guided Optimization of Energy Systems** – Nick Sahinidis
- **NMPC for Mode-Switching Operation of Reversible Solid Oxide Cell Systems** – Doug Allan, Michael Li
- **Optimal Long-Term Operation of Solid Oxide Electrolyzers considering Physical and Chemical Degradation** – Nishant Giridhar
- **Optimization-based Design Approaches for Rapid Deployment of Industrial Decarbonization Processes** – Georgia Stinchfield
- **Optimization for Infrastructure Planning of Reliable and Carbon-neutral Power Systems: Application to San Diego County** – Seolhee Cho

PARETO:

- **AquaTrade: The PARETO-Powered Produced Water Matchmaking Portal** – Philip Tominac
- **A Computational Framework to Evaluate Opportunities for Recovery of Rare Earth Elements and Critical Minerals in Produced Water Networks** – Arsh Bhatia
- **Project PARETO: A Systems Approach to Produced Water Management - From Advanced Infrastructure Buildout, Optimization, and Hydraulic Analysis to Treatment and Beneficial Reuse Across Industries** – Elmira Shamlou, Travis Arnold

PrOMMiS:

- **Designing Operationally Flexible Diafiltration Membrane Systems for Li/Co Separation** – Jason Yao
- **Opportunities for Membranes to Enhance Critical Mineral Processes** – Molly Dougher
- **PrOMMiS Unit Model Library** – Alejandro Garciadiego
- **Recycling Rare Earth Elements from End-of-Life Electric and Hybrid Electric Vehicle Motors** – Chris Laliwala
- **Science-Based Design of Experiments and Pyomo.DoE** – Hailey Lynch, Jialu Wang

OLI:

- **OLI Software: Thermodynamic Modeling Tool for Critical Materials** – Gaurav Das
- **OLI Automation: Cloud Thermodynamic Modeling Tools** – Adi Bannady
- **Predictive Chemistry Modeling in Carbon Capture, Transport, and Storage** – Leslie Miller
- **Scale Management and Mitigation Utilizing a Novel Theoretical Tool** – Gaurav Das

Supercritical CO_2:

- **Optimal Design of Power Cycles With Storage for Flexible Operation in High Variable Renewable Energy Electricity Markets** – Tyler Jaffe, Radhakrishna Tumbalam Gooty

WaterTAP:

- **Adsorption Processes in WaterTAP** – Hunter Barber, Kurby Sitterley
- **Crystallization Processes in WaterTAP** – Mayo Amusat, Zhuoran Zhang
- **Electrochemical Processes in WaterTAP** – Xiangyu Bi, Srikanth Allu
- **Evaporative Processes in WaterTAP** – Carson Tucker, Elmira Shamlou
- **Graphical User Interface for WaterTAP** – Dan Gunter, Michael Pesce
- **Industry Standard Biological Wastewater Treatment in WaterTAP** – Marcus Holly, Chenyu Wang
- **Multiperiod Modeling for Solar Driven and Flexible Desalination** – Mukta Hardikar, Akshay Rao
- **Osmotic Processes in WaterTAP** – Zach Binger, Chenyu Wang

For questions about agenda content and planning, please contact:

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