SSAE Newsletter

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// ABOUT

The Strategic Systems Analysis and Engineering (SSAE) directorate provides the decision science and analysis capabilities necessary to evaluate complex energy systems. The directorate's capabilities address technical, economic, resource, policy, environmental and market aspects of the energy industry. These capabilities are critical to strategic planning, direction and goals for technology R&D programs and the generation of market, regulatory and technical intelligence for NETL senior management and DOE. SSAE offers a range of multi-criteria and multi-scale decision tools and approaches for this support:

- Process systems engineering research: advanced modeling, simulation and optimization tools for complex dynamic systems
- Process and cost engineering: plant-level synthesis, process modeling and simulation of energy systems with performance estimates
- Resource and subsurface analysis: evaluation of technologies, approaches and regulations for subsurface energy systems and storage
- Market and infrastructure analysis: economic impacts and program benefits
- Environmental life cycle analysis: cradle-to-grave emissions and impacts

These tools and approaches provide insights into new energy concepts and support the analysis of energy system interactions at the plant, regional, national and global scales.

// HIGHLIGHTS

Update to the CO2_T_COM Released

An update to one of SSAE's open-source carbon capture, utilization and storage (CCUS) models and its associated user's manual was recently released. Developed by NETL, the FECM/NETL CO_2 Transport Cost Model is an Excel-based tool that estimates the costs for transporting liquid carbon dioxide (CO_2) by pipeline from a source (i.e., electric power plant or industrial plant) to either a CO_2 saline storage site or a CO_2 enhanced oil recovery site. The model, also known as CO2_T_COM, has a flexible interface that allows users to tailor the model to fit specific project requirements and calculate revenues and capital, operating and financing costs as well as the break-even cost (in $/tonne) for a project transporting CO_2 by pipeline (learn more).

In addition to some formatting changes throughout the model and corrections to some minor errors discovered in the previous version, a new equation was added to calculate natural gas pipeline capital costs per a 2022 study by Brown et al. along with a method for calculating average costs for all the regions in the United States. Modeling of decarbonization scenarios indicate that CCUS is expected to play a critical role in meeting net zero goals by 2050. Analytical tools, like the CO2_T_COM, that can provide valuable quantitative cost and performance insights given interrelationships amongst essential technologies, enabling policies and prevailing regulations will remain critical decision support resources for widespread deployment of CCUS. The CO2_T_COM can help evaluate integrated CCUS networks (i.e., connecting a CO_2 source to a storage site) and costs of large-diameter trunkline or shorter, smaller pipelines (e.g., gathering/distribution).

Want to learn more about SSAE's work?

Click here to see previous SSAE newsletter issues

Staff Spotlight

Mike Marquis* is a geologist and modeler, with over 20 years of experience, who specializes in constructing highly-specialized, quantitative geographic information system (GIS) models of upstream and downstream energy systems. His prior professional experience working at Advanced Resources International and Enegis, LLC encompassed a wide variety of energy sectors including CCUS.

Mike has a B.S. in Geology from the College of William and Mary. He lives in the northern Shenandoah Valley of Virginia with his two small children.

* NETL Support Contractor

// NOTICES

SSAE Welcomed Mickey Leland Scholars

This summer SSAE welcomed five students to work under its process and cost engineering, markets, subsurface and process systems engineering competencies as part of the Mickey Leland Energy Fellowship (MLEF) summer educational fellowship program. This highly competitive ten-week program for students in science, technology, engineering and math majors provides scholars the unique opportunity to gain direct research experience with carbon management/resource sustainability at various DOE national laboratories. At NETL, students research onsite for nine weeks before a one-week, offsite technical forum. Background on the five MLEF scholars and their research projects is provided below.

Sydney Cohen is a third-year student at Brandeis University majoring in computer science and environmental studies. She is an Undergraduate Departmental Representative for the Computer Science Department and has worked as a teaching assistant for Advanced Programming Techniques in Java. She is also the event-coordinator of Students for Environmental Action. Sydney was a research assistant studying the international conservation of migratory species in North America, working to collect and analyze data on individual species to improve the understanding of existing governance structures. She is interested in using computing to support climate solutions and infrastructure, especially in the energy, transportation and natural disaster sectors. In her free time, she loves spending time with her two cats. Sydney also enjoys running and exploring the outdoors, along with cooking, 3D printing and reading.

Biomass with carbon capture and storage (CCS) is a promising hydrogen production method that could have high associated water risks. To implement hydrogen production from biomass gasification with CCS, it is important to identify regions with high water availability, low water risk and an adequate supply of biomass. Working with SSAE's Alison Fritz, Sydney assessed regional tradeoffs between water availability and hydrogen production methods in the United States. As part of her research project she 1) completed a literature review, which indicated potential biomass sources and evaluated their sustainability; 2) cleaned and aggregated water risk, greenhouse gas emissions and cropland datasets; 3) developed a Jupyter Notebook in Python with the Pandas library to identify regional tradeoffs between water use and hydrogen energy generation; 4) analyzed crop production as a source for biomass at a national level using water sources as the primary constraint; 5) classified and mapped difficult-to-electrify high-emissions industries that may be promising regions for hydrogen use (namely glass production, ammonia manufacturing, cement production, iron and steel production and petroleum refining); 6) examined the water need and intensity of hydrogen energy from biomass gasification compared to that of other fossil energy sources and 7) looked at variation in water demand depending on the type of crop used.

Sean Franco is an applied economics graduate student at The George Washington University. He is an aspiring environmental economist and data scientist. Sean has prior work experience in standardized testing, land surveying and social justice and education policy. He has four years of research experience including field work, data analysis and professional research presentations. Sean is a member of Citizen's Climate Lobby and a past co-leader of an URGE podlet. In his spare time, Sean plays old-time fiddle music and likes to read.

The objective of Sean's research project was to examine how the Inflation Reduction Act's prevailing wage and apprenticeship (PWA) requirements might influence the economics of a firm's decision to invest in carbon capture technologies. Focusing on entities that would be eligible for the Carbon Oxide Sequestration (i.e., Section 45Q) tax credit and using data from NETL's Baseline Studies for Fossil Energy Plants, Sean, working with SSAE's Amanda Harker Steele, conducted scenario and other analyses to assess how the costs of electric generating units are influenced by the PWA requirements. These requirements stipulate the wages that laborers, mechanics, contractors and sub-contractors must be paid and the percentage of total labor hours for construction, alteration or repair work that must be performed by a qualified apprentice. They also allow eligible entities to receive five times the base value of the Section 45Q credit per unit of CO_2 that is captured and stored. Executing this project enhanced Sean's programming skills and taught him the economics of electric generating units.

Brandon Colon just finished a bachelor's degree in computer engineering at the University of Texas San Antonio and is eager to begin a graduate degree in aeronautical engineering after serving as an Infantry Solider for the Texas Army National Guard.

Brandon spent the summer working with SSAE's Eric Liese on a research project with the objective of finding a convenient source of year-long hourly weather data for any location as this data could be useful for NETL researchers in various techno-economic analyses. For example, a direct air capture system's effectiveness is dependent on ambient dry bulb temperature and humidity. Power cycles can also be strongly impacted by these conditions. Typically, international standard or location average ambient conditions are assumed; however, analyses could make use of more refined year-long hourly conditions. Brandon used Python within a Jupyter Notebook to download the data via an API hosted by the National Aeronautics and Space Administration's Global Modeling and Assimilation Office. The weather data is an assimilation of various data sources and is labeled Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2). Brandon wrote a document that summarized the program and the MEERA-2

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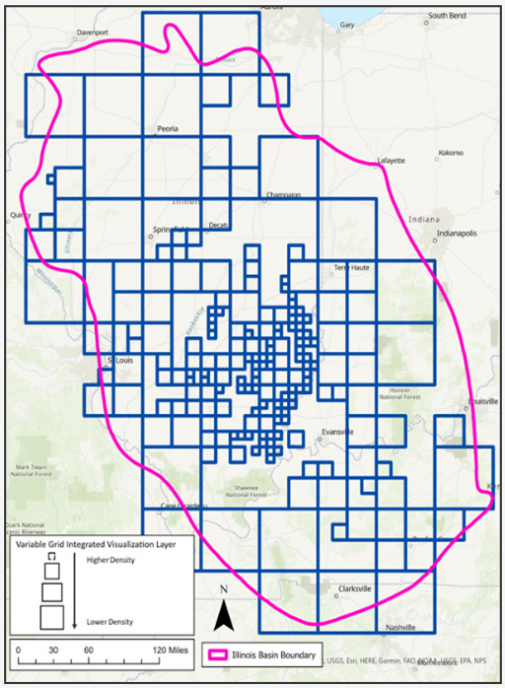
data. He also wrote a Python application which demonstrates the translation of the unique data file type (nc4) into a Python data frame and csv file after which some interesting statistical analyses were performed. Brandon presented his work to SSAE's Process Systems Engineering Research Team and at the MLEF final meeting in Washington D.C. Brandon's hard work and enthusiasm resulted in the development of a useful tool for NETL researchers.

Araceli Lara is a 2023 graduate of the University of Portland with a B.S. in Environmental Science and Sustainability.

Working with SSAE's MacKenzie Mark-Moser on her research project, Araceli examined spatial methods for assessing data availability to support the EDX4CCS Field Work Proposal's Task 21, which focuses on determining the technical viability of carbon storage in sedimentary systems. In this project, she used the Variable Grid Method to assess density of well data in the Illinois Basin.



Carly Fowler is a rising junior at Duke University, pursuing a degree in mechanical engineering. Carly is passionate about carbon capture and hopes to make this a focus in her future career. She is fascinated by the relationship between public policy, science and technology and their collective impact on energy transition. On campus, Carly participates in the Duke University Undergraduate Energy Club, which provides her with educational experiences and professional networking opportunities. As a member of the club, she completed a hydropower market research project for Rye Development, LLC and a geothermal value chain analysis for Quaise Energy. Last semester, Carly performed research on rock characterization for CO_2 sequestration and geothermal applications. In her free time, she loves to dance and spend time with her friends and family at the beach.

Coal mining and production have declined in the United States resulting in thousands of abandoned mines. Working with SSAE's John Brewer, Carly researched the potential to use these abandoned mines for renewable energy. During her research, Carly found mine pools could be repurposed. Mine pools form when groundwater floods the mine shafts after operations have ended. Each mine pool can store over a billion gallons of water, making them great resources for renewable energy such as hydropower and geothermal heat pumps. Carly's primary goal was identifying ways to repurpose mine pools as a means to revitalize communities impacted by legacy coal mining. She created a priority list of economically distressed communities, explored hydropower and geothermal heat pumps and researched the policies regulating the mines. This introductory work exposed a need to create a more comprehensive database for abandoned mines. There is limited information on the structure, water storage capacity and water quality of mine pools that, if available, would be essential to implementing renewable energy systems.

PARETO Team Presents at Texas Produced Water Consortium Conference

The technical team of Project PARETO—DOE's produced water optimization initiative—traveled to Austin, TX, to present project updates to stakeholders at the Texas Produced Water Consortium's annual conference in August 2023. The meeting attracted attendees from across the produced water community including industrial practitioners, government and regulatory agencies and academic researchers. The meeting featured presentations on topics such as produced water treatment technologies, produced water characterization and monitoring tools and legislative updates from Texas State Senator Charles Perry.

The PARETO team presented for two hours, giving updates on the team's progress on modeling beneficial reuse options, hydraulics and desalination technologies for produced water from onshore oil and gas operations. The presentation featured a demo of PARETO's graphical user interface, which focused on highlighting PARETO capabilities for produced water management and infrastructure build-out optimization, and risk assessment (by solving what-if scenarios). PARETO's source code is available on GitHub, and the accompanying graphical user interface is available for download as open-source software. Documentation of the PARETO framework is also available online.

Finally, the team introduced AquaTrade, a new tool developed in collaboration with the Ground Water Protection Council. AquaTrade is an open platform to aid operators in identifying mutually beneficial water sharing arrangements. The aim of this tool is to help operators intensify existing water sharing practices, thereby increasing water recycling rates and reducing freshwater consumption required for oil and gas operations

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PARETO Team members attending the meeting, pictured from left to right, are Karen Work (Lawrence Berkeley National Laboratory [LBNL]), Melody Sherman*, Travis Arnold*, Markus Drouven, Vanessa Núñez-Lopez (DOE-HQ), Elmira Shamlou*, Miguel Zamarripa*, Philip Tominac*, Michael Pesce (LBNL) and Naresh Susarla*, not pictured Lisa Henthorne (LBNL).

SSAE Researchers Discuss Various Topics at FECM/NETL Meeting

Several SSAE staff joined NETL's Acting Director Sean Plasynski and other NETL experts to showcase their research at the 2023 FECM/NETL Carbon Management Research Project Review Meeting in August 2023. The meeting featured presentations on point source carbon capture, carbon dioxide removal (CDR), carbon conversion and carbon transport and storage and was co-located with the United States Energy Association's inaugural Carbon Management Technology Showcase. Listed below are the SSAE presentations, posters and demonstrations. Publication is pending for several presentations/posters, as noted below.

CO_2 Removal

- An overview of completed and ongoing SSAE work in the CDR area was presented by Timothy Fout. The presentation, "Systems Analysis for Carbon Dioxide Removal" (pending publication), covered several topics including direct air capture, marine CDR and enhanced weatherization along with preliminary highlights on markets and life cycle analysis (LCA) work in the area. The LCA work discussion focused on bio-energy with CCS/biomass with carbon removal and storage.
- Details of the design basis of NETL's active work on the techno-economic analysis of enhanced weathering and marine CDR was highlighted by Sarah Leptinsky* in a poster presentation, "Techno-economic Analysis Development for Enhanced Weathering and Marine Carbon Dioxide Removal Case Studies." Enhanced weathering is the acceleration of the natural weathering of alkaline rocks by spreading finely ground rocks onto surfaces to facilitate chemical reactions between rocks and CO_2. Marine CDR is indirect CDR from the atmosphere via an enhancement of the downward air–sea flux of CO_2 from the atmosphere to the ocean surface.

CO_2 Conversion

- A demonstration of the NETL CO2U LCA Guidance Toolkit was given by Michelle Krynock and Joseph Chou*. This toolkit includes the NETL CO2U LCA Guidance Document, NETL CO2U openLCA LCI Database, NETL CO2U openLCA Results Contribution Tool, NETL CO2U LCA Documentation Spreadsheet and NETL CO2U LCA Report Template.

Point Source Carbon Capture

- An overview on uncertainty quantification and technical risk reduction workflows developed in the Carbon Capture Simulation for Industrial Impact ($CCSI^2$) project was highlighted by Chrysanthos Gounaris* in a presentation summarizing a report co-authored by Alex Dowling*, "Technical Risk Reduction: Model Based Design of Experiments and Robust Optimization" (pending publication). This presentation focused on intrusive methods that exploit structure information from model equations with applications in point source capture. Most modeling efforts start with a mathematical model based on science and engineering fundamentals (e.g., thermodynamics, transport) from experiment data. The first step in uncertainty mitigation is estimating parameters in these models such as rate or equilibrium constants. Next, sequential model-based design of experiments (SMBDoE) is used to optimize future experimental campaigns to reduce parameter uncertainty or discern between alternative models. Finally, robust optimization determines the best designs (e.g., minimize costs) while considering how model and operational uncertainty impacts performance (e.g., maintain high CO_2 capture rates).
- An overview of the computational guidance for RTI International (RTI) Technology Centre Mongstad (TCM) test campaign, including the successes of the ongoing collaboration between the $CCSI^2$ program and RTI, was presented by Joshua Morgan. This presentation, "Computational Guidance for RTI TCM Test Campaign" (pending publication), discussed the sequential design of experiments (SDoE) tools developed by $CCSI^2$ that were applied to support the generation of a high-quality data set for RTI's non-aqueous solvent (NAS) CO_2 capture system in a test campaign at TCM. The results of this campaign demonstrated the promise of this system as a novel capture technology due to its ability to capture high levels of CO_2 with reduced energy penalty in comparison to baseline systems. The presentation also included an overview of the ongoing modeling and uncertainty quantification efforts, along with the plan for $CCSI^2$ to provide process and property modeling support for the development of the next-generation technology in RTI's NAS solvent class in a new DOE-funded project.
- Primary takeaways from two reports that were recently released by NETL on retrofitting natural gas combined cycle (NGCC) and pulverized coal (PC) power plants with solvent-based carbon capture technology was featured in a poster presentation given by Gregory Hackett. This poster, "Retrofitting NGCC and PC Power Plants with Carbon Capture Technology," focused on the performance and cost of retrofitting these plants at 90 and 95% carbon capture, including consideration of cases that attempt to make up for steam turbine derates caused by extracting steam for use in the capture process. Additionally, the poster highlighted NETL's recently released carbon capture retrofit databases (CCRD) for both NGCC and PC plants. The CCRDs are public-

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facing tools that allow the end-user to approximate the incremental cost of CO_2 capture for a user-defined plant with retrofitted capture technology.

- A study evaluating the cost of capturing CO_2 from a 400,000 air dried tonne/year pulp production plant using Shell's CANSOLV post-combustion capture process and considering greenfield and retrofit cases was featured in a poster presentation, "Techno-economic Analysis of CO_2 Capture from Pulp/Paper Plants," given by Hari Mantripragada*. Pulp and paper plants are unique among industrial emitters as there is sufficient steam and electricity available from the base plant itself to meet the capture system demands in greenfield applications, making their cost of CO_2 capture much lower than retrofit cases, which produce steam from an auxiliary natural gas boiler and purchase power from the grid.
- A study focusing on the temperature vacuum swing adsorption (TVSA) process and sweep gas for regeneration was featured in a poster presentation given by Daison Yancy Caballero*. This poster, "Process Modeling and Analysis of a Novel Sorbent Material for Direct Air Capture Applications" (pending publication), discussed assessing the feasibility for direct air capture of PIM-1-AO-TAEA NETL sorbent, both simplified and rigorous adsorption cycle models were developed using the Institute for Design of Advanced Energy Systems (IDAES) and Aspen Plus®.

Carbon Transport and Storage

- The status and accomplishments of Task 5 of Phase 3 of the National Risk Assessment Partnership (NRAP) was highlighted by David Morgan in a presentation titled "Task 5: Developing a Tool to Quantify Liability of Geologic Carbon Storage" (pending publication). This task involves examining the costs associated with responding to adverse events at a CO_2 saline storage site, specifically the cost of responding to leakage of CO_2 and brine out of the storage formation into an underground source of drinking water or the cost of responding to induced seismic incidents. The task involves modifying the Python version of the FECM/NETL CO_2 Saline Storage Cost Model to account for the costs of responding to these two types of adverse events and using these costs to estimate the liability associated with these adverse events.
- An overview of the geoanalytical economic evaluation of saline storage (GEESS) system was featured in a presentation, "GEESS as a Mechanism to Facilitate the Commercialization of Geologic Carbon Sequestration (GCS)" (pending publication), given by Jeffrey Eppink* and co-authored by Austin Matthews*. The GEESS model is currently undergoing development and currently characterizes 57 geologic saline formations in the lower-48 states. It incorporates discrete data for each formation including formation name, state, basin, lithology, depositional environment, geologic age, area of analysis, grid point latitude and longitude, drill depth, thickness, reservoir pressure and temperature, porosity, permeability, salinity, structural regime classification and fracture pressure. The acquisition, aggregation and processing of these data enables the GEESS system to be suitable as a mechanism to facilitate the commercialization of geologic carbon sequestration. Accordingly, it can provide a standardized, rigorous, detailed platform that is compatible with the FECM/NETL CO_2 Saline Storage Cost Model, a capability to be used as an exacting screening tool for carbon sequestration project suitability and a viable assessment tool for research and development impacts.
- An overview of the recent offshore Gulf of Mexico (GoM) CCS project announcements and improvements in project economics attributable to 45Q and to the regulatory landscape with project advancements was presented by Connie Zaremsky*. This presentation, "Recent Developments in Deployment of CCS Projects in the Offshore Gulf of Mexico" (pending publication), also examined the remaining hurdles to potentially broader CCUS deployment in the offshore GoM. During last year's 2022 FECM/NETL Carbon Management Project Review Meeting, NETL presented an analysis that identified potential economic and regulatory barriers to CCUS project deployment in the offshore GoM. Coincidentally, in that same week, the economics for CCUS were significantly improved with the passage of the Inflation Reduction Act (IRA) which extends and expands the 45Q tax credit. In the last year, since the passage of the IRA, there have been over 70 new CCUS project announcements in the United States, about a 30% increase over last year.
- A database on technically viable CCS resources assessment was discussed in a presentation given by Christopher Creason and co-authored by MacKenzie Mark-Moser. This presentation, "Carbon Storage Technical Viability Approach" (pending publication), highlighted ongoing work to develop a database, evaluation criteria and workflow that integrates additional factors beyond technically recoverable storage resources to inform and accelerate technically viable carbon storage assessments in the United States.
- The analysis of biomass power production with CCS pathways was the focus of a poster presentation given by Roksana Mahmud* and Jorge Izar-Tenorio*. This poster, "Biomass Environmental Analysis in Bioenergy with Carbon Capture and Storage Modeling" (pending publication), discussed a tool for examining emissions potentials, water consumption and scarcity and land use for various biomass types co-fired with coal and equipped with saline aquifer carbon storage.
- The background, methodology and results of a case study prototyping interactions between NRAP tools and the FECM/NETL CO_2 Saline Storage Cost Model to quantify the costs associated with responding to an environmental adverse event was provided in a poster, "A Framework for Linking Quantitatively Assessed Risks and Costs for Geologic Carbon Storage (GCS) to Consider Impact of Contingency Plans at a GCS Site" (pending publication), presented by Travis Warner* and co-authored by Derek Vikara* and David Morgan.
- An economic analysis assessing CCS networks in the Central United States was the focus of a poster presentation,

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"Comparative Economic Analysis of Capture, Transport, and Storage from a CO_2 Source Perspective in the Central U.S." (pending publication), given by Alana Sheriff*. The study focused on three defined regions within the Central United States and used NETL-developed models and resources to estimate overall CCS costs (capture, transport and storage) in $/tonne. Four source types with a range of CO_2 capture rates, seven source locations, eight saline storage reservoirs and two pipeline transportation options were modeled, resulting in the evaluation of over 100 integrated source-to-sink matching scenarios.

- An overview of the techno-economic models NETL has developed for assessing performance characteristics and cost drivers for CO_2 pipeline transport, CO_2 saline storage and oil production and CO_2 storage using CO_2 enhanced oil recovery was provided in a poster presentation given by Derek Vikara*. This poster, "NETL's Techno-Economic Modeling Resources for Analyzing Decarbonization Strategies using CCUS" (pending publication), also provided a high-level description of each model along with useful outputs that can be generated with each model. NETL has developed techno-economic models to evaluate the performance characteristics and costs for each component of the CCUS value chain: CO_2 capture, transport and geologic storage. These tools can be used individually to evaluate the economic opportunity for specific CCUS components, or they can be used in tandem to assess integrated CCUS systems.
- A review of the general requirements for geological input data to support assessment of CO_2 storage options at various scales was highlighted in a poster presentation given by Ray Boswell. This poster, "Geologic Storage Assessment Review: Focus on Appalachia" (pending publication), featured a comparison of these expectations to the current content of publicly available National Carbon Sequestration Database and Geographic Information System (NATCARB) databases, with primary focus on potential Appalachian saline and oil and gas reservoirs. Initial results of new mapping efforts were also provided that relate to potentially undervalued Appalachian reservoir options in Upper Devonian sandstones and overpressured shales.
- A demonstration of the CO_2 Capture, Transport and Storage (CTS) Screening Tool, a cost screening tool that identifies cost-optimal transport and storage scenarios and their associated CTS costs from the perspective of a CO_2 point source engaged in CCS or CCUS, was provided by Taylor Vactor*. The tool leverages results databases derived from a variety of NETL's publicly available transport and storage cost modeling tools and capture cost reports. Developed by Travis Warner*, Alana Sheriff* and Mike Marquis*, this tool is not yet publicly available.

// PERSPECTIVES

DOE's Water treatment Technoeconomic Assessment Platform (WaterTAP)

SSAE researchers are leading the development of WaterTAP, an open-source software tool for evaluating water treatment technologies. This work is funded by DOE research programs under the Industrial Efficiency and Decarbonization Office (IEDO), the Solar Energy Technology Office (SETO) and the National Alliance for Water Innovation (NAWI) which is DOE's desalination hub. The common goal of these research programs is to advance technologies to support a circular water economy, where water is repeatably reused with fit-for-purpose treatment and contaminants are recovered as valuable products.

WaterTAP supports advancing water treatment technologies by providing a platform to conduct detailed technoeconomic assessments. These analyses enable researchers to identify innovation opportunities, determine technological bottlenecks and set research targets for new materials, components and processes by quantifying performance and cost metrics. WaterTAP provides this capability by developing a modular model library for a wide range of water treatment technologies and is built on an advanced process systems engineering platform developed and led by NETL called IDAES, which won the R&D 100 award in 2020. IDAES provides WaterTAP with a strong computational capability for assembling the developed modular models to represent water treatment trains and for supporting analyses through simulation and optimization. WaterTAP seeks to be more unified, flexible and powerful than current water treatment software by being open-source, modular, multi-hierarchical, customizable and equation oriented. Additional background on these attributes, as well as more discussion on the funding research programs, can be found in the November 2022 SSAE Newsletter.

The WaterTAP development team, which primarily consists of members from five national labs including NETL, LBNL, National Renewable Energy Laboratory, Oak Ridge National Laboratory and SLAC National Accelerator Laboratory, has developed an extensive library of water treatment models. These models are organized in three categories: 1) unit models that relate equipment performance to its design and operating variables, 2) property models that relate water properties to the state variables and 3) cost models that relate capital and operating costs to the system design and operating variables. Unit operations that can be represented on WaterTAP include:

// PERSPECTIVES (cont'd)

- Membrane/osmotic processes – nanofiltration and reverse osmosis (RO) including emerging modifications like high pressure RO, low-salt-rejection RO and osmotically assisted RO
- Electrochemical processes – electrodialysis, electrocoagulation and electrolyzers for base and acid generation
- Evaporative processes – mechanical vapor compression, multi-effect distillation and membrane distillation
- Ad/absorptive processes – granular activated carbon and ion exchange
- Chemical processes – chemical precipitators and pH control
- Biological processes – activated sludge and anaerobic digestors

Besides providing simulation and optimization capabilities for conducting technoeconomic assessments, WaterTAP offers several other utilities to support and expand analyses:

1. A parameter sweep tool that enables users to seamlessly conduct single and multiple parameter sensitivities, manage the results and create figures. This WaterTAP tool was demonstrated in a published study on an emerging multistage membrane process called low-salt-rejection RO, where the levelized cost of water was assessed across its full application and involved thousands of individual cost optimal solutions (see Figure 1).
2. A graphical user interface that enables users to visualize flowsheets and explore the effect of varying key parameters and variables. This interface requires the initial model to be built through a code-based interface, but then it can be shared with non-coding users.
3. A parameter estimation capability that allows users to fit parameters in a mechanistic model to experimental data. This capability is directly from IDAES and its previous development.
4. A surrogate modeling capability that allows users to create a model from experimental data. These models can be based on regression, radial basis functions (interpolation like method), Kriging or machine learning. Similarly, this capability is directly from IDAES and its work with the surrogate modeling tools ALAMO and PySMO.
5. A multiperiod modeling capability that automates the creation of multiple instances of steady state models that can be connected to make a pseudo-steady state model to represent how the process performs over time. This capability was leveraged from another SSAE led project called DISPATCHES that, like WaterTAP, was built off the IDAES platform.

Over the past two and a half years, the WaterTAP team has publicly released updated versions of WaterTAP every quarter. The most recent version, WaterTAP V0.9, was released in June 2023. While the WaterTAP team primarily focused on building the platform during its first two years, the team is now focused on using the tool to conduct analyses and currently has two manuscripts under review and three more in preparation. These manuscripts cover a range of water treatment technologies including osmotic, evaporative, ad/absorptive and electrochemical processes. This year, the WaterTAP team has also been collaborating with three IEDO wastewater resource recovery projects and analyzing solar driven desalination technologies for SETO. Additionally, the WaterTAP team has planned or kicked off seven new collaborations with NAWI research projects and pilot-scale demonstrations.

WaterTAP development is currently funded through December 2024. If NAWI (DOE's desalination hub) is renewed for another five years, it is expected that WaterTAP funding will be extended through December 2029. In the long-term, WaterTAP developers will assess opportunities for supporting more water treatment models and advanced computational capabilities which could include dynamic modeling, mixed-integer programming, conceptual design, uncertainty quantification, stochastic programming and robust optimization. Besides providing value to the funding research programs, WaterTAP's mission is to provide the broader water research community with an integrated, open-source modeling and simulation capability to help researchers advance water treatment technologies.

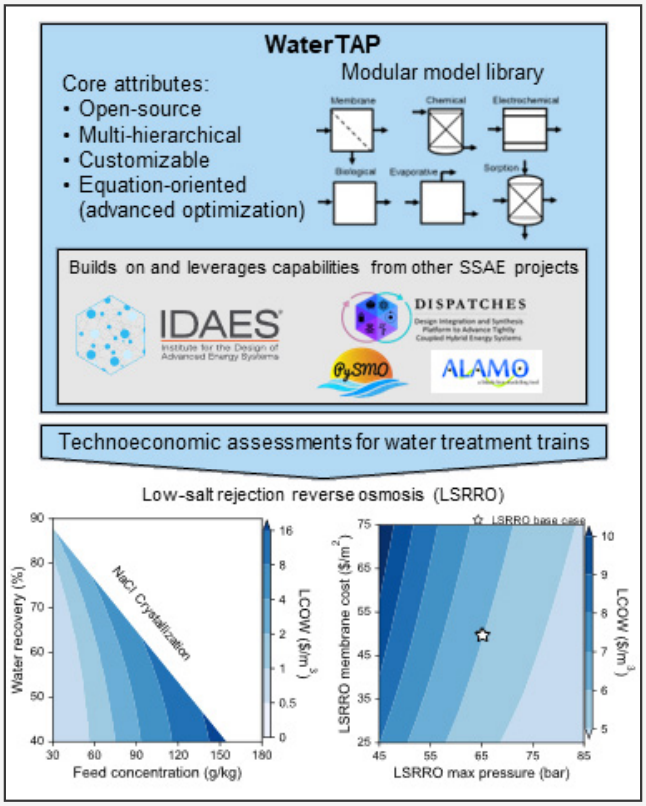

Figure 1. Schematic visualizing the key components of WaterTAP and the other SSAE projects it builds on. Technoeconomic assessment results are shown for low-salt-rejection RO, an emerging multi-stage membrane process. Both plots show the levelized cost of water (LCOW) as a function of key parameters. The plot on the left analyzes the system across its application space for different feed concentrations and water recoveries. The plot on the right analyzes the system for one case (100 g/kg feed concentration and 50% water recovery) across two membrane parameters – the maximum allowable operating pressure and its cost.

// UPCOMING CONFERENCES AND EVENTS

SSAE federal staff and NETL support contractor personnel will attend or present at the following conferences in September 2023:

- Utah FORGE 2023 R&D Annual Workshop
  Participant: MacKenzie Mark-Moser
  Virtual, September 7–8, 2023
- Groundwater Protection Council 2023 Annual Forum
  Presenters: Markus Drouven – A Produced Water Sharing Framework to Promote Water Reuse in Oil and Gas Operations and Philip Tominac* – PARETO (software demonstration)
  Tampa, FL, September 12–14, 2023
- NERC Energy Assurance with Energy-Constrained Resources Standards Drafting Team Meeting
  Participant: John Brewer
  Virtual, September 14, 2023
- 7th Post Combustion Capture Conference (PCCC-7)
  Presenter: Ashley Cutshaw*; Timothy Fout – 1) Examination of Factors Affecting the Cost and Performance of NGCC with CCS and 2) Technoeconomic Analysis of Sorbent-based Direct Air Capture and Sally Homsy* – Insights from FEED Studies for Retrofitting Existing Fossil Power Plants with Post Combustion Capture Technology
  Participants: Robert James and Benjamin Omell
  Pittsburgh, PA, September 25–27, 2023
- American Center for Life Cycle Assessment (ACLCA) 2023 Conference
  Presenters: Matthew Jamieson – U.S. Department of Energy Special Session; Megan Henriksen* – Life Cycle Analysis of Synthetic Natural Gas Production via Carbon Conversion: Impact of Different CO_2, H_2, and Methanation Pathways; Roksana Mahmud* – Towards a Sustainable LCA Framework for Critical Mineral Production in the U.S. and Sheikh Moni* – National Energy Technology Laboratory CO_2 Utilization (CO2U) Life Cycle Analysis (LCA) Toolkit: Overview, Applications and Recent Updates
  Participant: Michelle Krynock
  Burlington, VT, September 25 (pre-conference workshops) and 26–29 (conference), 2023
- Electric Power Transformation: 2023 MEGA Symposium
  Presenter: Gregory Hackett – Carbon Capture Technologies: Status and Challenges
  Panelist: Peter Balash – Plenary Session: Key Issues for Clean and Reliable Energy
  Pittsburgh, PA, September 26–27, 2023

// RECENT PUBLICATIONS

Articles

- Z. Wu, H. Zhai, E. Grol, C. Able and N. Siefert, "Treatment of brackish water for fossil power plant cooling," *Nature Water*, vol. 1, pp. 471-483, May 22, 2023.
- M. Henriksen, H. S. Matthews, J. White, L. Walsh, E. Grol, M. Jamieson and T. Skone, "Tradeoffs in life cycle water use and greenhouse gas emissions of hydrogen production pathways," *International Journal of Hydrogen Energy*, August 24, 2023.
- R. Newby, D. Keairns and R. Stevens, "Chemical looping combustion oxygen carrier production cost study," *Applied Energy*, vol. 345, article 121293, September 1, 2023.
- C. Able, D. Rellergert, Mazzoni and E. Grol, "Assessment of combustion residual leachate volume, composition, and treatment costs," *Journal of Hazardous Materials*, vol. 457, article 131731, September 5, 2023.

Book Chapter

- A. Cutshaw, J. Chou, T. Skone, M. Krynock, and M. Jamieson, "Life Cycle Analysis of Thermoelectric Power Generation in the United States", in Encyclopedia of Sustainable Technologies – Power LCA Update, Elsevier, 2023.

* NETL Support Contractor

// RECENT PUBLICATIONS cont'd

Models/Tools/Databases

- National Energy Technology Laboratory, "Autothermal reforming (ATR) operations with carbon capture (CCS)," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Biomass and coal gasification operations with carbon capture (CCS)," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Biomass gasification operations," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Coal gasification operations," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Coal gasification operations with carbon capture (CCS)," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Polymer Electrolyte Membrane (PEM) electrolysis system construction," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Polymer Electrolyte Membrane (PEM) operations," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Solid Oxide Fuel Cell (SOEC) operations," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Steam Methane Reforming (SMR) operations," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Steam Methane Reforming (SMR) operations with carbon capture (CCS)," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.
- National Energy Technology Laboratory, "Energy Cane Cultivation," National Energy Technology Laboratory, Pittsburgh, PA, January 2023.
- National Energy Technology Laboratory, "Hybrid Poplar Cultivation," National Energy Technology Laboratory, Pittsburgh, PA, January 2023.
- National Energy Technology Laboratory, "Cement production with optional carbon capture," National Energy Technology Laboratory, Pittsburgh, PA, March 2023.
- National Energy Technology Laboratory, "FECM/NETL CO_2 Transport Cost Model (2023)," Version 4, National Energy Technology Laboratory, DOE/NETL-2023/4384, Pittsburgh, PA, July 26, 2023.

Reports/Supporting Documentation

- Z. Wu, H. Zhai, E. Grol, C. Able and N. Siefert, "Treatment of brackish water for fossil power plant cooling – Supporting Information," May 22, 2023.
- S. Leptinsky, T. Schmitt, A. Zoelle, S. Homsy, M. Woods, T. Shultz and J. Hoffmann, "Cost and Performance Projections for Coal- and Natural Gas-Fired Power Plants," National Energy Technology Laboratory, DOE/NETL-2023/4382, Pittsburgh, PA, May 31, 2023.
- D. Morgan, A. Guinan and A. Sheriff, "FECM/NETL CO_2 Transport Cost Model (2023): Description and User's Manual," National Energy Technology Laboratory, DOE/NETL-2023/4385, Pittsburgh, PA, July 26, 2023.
- C. Able, D. Rellergert, V. Mazzoni and E. Grol, "Assessment of Combustion Residual Leachate Volume, Composition and Treatment Costs (Supplementary Information)," September 5, 2023.

Presentations

- E. Shuster, "2023 Water Brief for Energy Applications," National Energy Technology Laboratory, Pittsburgh, PA, 2023.

Conference Proceedings and Events

- M. Zamarripa, R. Gooty and J. Eslick "IDAES Workshop Introduction," IDAES Workshop, Virtual, June 2, 2022.
- S. Min Choi Hong, E. Hedrick, K. Hedrick, D. Beahr, D. Bhattacharyya, S. Zitney and B. Omell, "Multiple And Nonlinear Model Predictive Control for Rapid Load-Following Operation of Supercritical Pulverized Coal Power Plants," presentation at the 2022 AIChE Annual Meeting, Phoenix, AZ, November 16, 2022.

// RECENT PUBLICATIONS cont'd

- G. Stinchfield, M. Zamarripa, J. Morgan and C. Laird, "Optimal Design Approaches for Rapid, Cost-Effective Manufacturing and Deployment of Chemical Processes," poster at the Center for Advanced Process Decision-Making (CAPD) Annual Review Meeting, Pittsburgh, PA, March 6, 2023.
- S. Pidaparti, C. White, E. Liese and N. Weiland, "Performance and Cost Potential for Direct-Fired Supercritical CO_2 Natural Gas Power Plants," 2023-sCO2.eu-116, presentation (conference paper) at the 5th European sCO_2 Conference for Energy Systems, Prague, Czech Republic, March 14–16, 2023.
- A. Bhatia, J. Pulsipher, D. Ovalle Varela, M. Zamarripa, M. Drouven and C. Laird, "A Framework for Evaluating and Optimizing Critical Mineral Recovery Opportunities in Produced Water Networks," presentation at the SPE Workshop: Full Life Cycle Management of Produced Water, Galveston, TX, May 23–25, 2023.
- S. Homsy and T. Fout, "Environmental Impact of Capture Technology: A Review of DOE-Sponsored FEED Studies," presentation at the USEA and FECM Workshop on Measurement, Monitoring and Controlling Potential Environmental Impacts from the Installation of Point Source Capture, Birmingham, AL, June 2023.
- H. Khutal, M. Blackhurst, N. Willems, H. S. Matthews, K. Chivukula, Priyadarshini, H. Hoffman, M. Jamieson and T. Skone, "Evaluating U.S. Natural Gas Environmental Performance," presentation at the International Symposium on Sustainable Systems and Technology (ISSST) 2023 Conference, Fort Collins, CO, June 14, 2023.
- S. Moni, J. Chou, M. Henriksen, J. Clarke and M. Krynock, "Life Cycle Analysis of Emerging Technologies: Overview and Updates of NETL CO2U LCA Toolkit" presentation at the International Symposium on Sustainable Systems and Technology (ISSST) 2023 Conference, Fort Collins, CO, June 14, 2023.
- S. Hughes, G. Hackett and E. Grol, "NETL's Carbon Capture Retrofit Databases," presentation at the 47th International Technical Conference on Clean Energy – The Clearwater Clean Energy Conference, Clearwater, FL, July 25, 2023.
- S. Hughes and E. Grol, "Analysis of Carbon Capture Retrofits for Cement Plants," presentation at the 47th International Technical Conference on Clean Energy – The Clearwater Clean Energy Conference, Clearwater, FL, July 25, 2023.
- J. Morgan, M. Campbell, K. Rao Putta, M. Ismail Shah, L. Herraiz-Palomino, S. Garcia Lopez, M. van der Spek, M. Matuszewski and B. Omell, "Modeling and Uncertainty Quantification of CESAR1 Solvent System for Post-Combustion Capture," presentation at the 47th International Technical Conference on Clean Energy – The Clearwater Clean Energy Conference, Clearwater, FL, July 25, 2023.
- G. Hackett, K. Buchheit, T. Schmitt, N. Kuehn, A. Zoelle, S. Homsy, M. Woods, T. Shultz and T. Fout, "Retrofitting NGCC and PC Power Plants with Carbon Capture Technology," poster at the 2023 FECM/NETL Carbon Management Research Project Review Meeting, Pittsburgh, PA, August 29, 2023.
- S. Leptinsky, T. Schmitt, S. Homsy, M. Woods and T. Fout, "Techno Economic Analysis Development for Enhanced Weathering and Marine Carbon Dioxide Removal," poster at the at the 2023 FECM/NETL Carbon Management Research Project Review Meeting, Pittsburgh, PA, August 29, 2023.
- H. Mantripragada, S. Hughes, A. Zoelle, E. Grol and T. Fout, "Techno-economic Analysis of CO_2 Capture From Pulp/Paper Plants," poster at the at the 2023 FECM/NETL Carbon Management Research Project Review Meeting, Pittsburgh, PA, August 29, 2023.
- E. Grol, "Overview of Industrial CO_2 Capture Analysis at NETL," presentation at the 2023 FECM/NETL Carbon Management Research Project Review Meeting, Pittsburgh, PA, August 31, 2023.

// REFERENCE SECTION

Models / Tools / Databases

Carbon Capture Simulation Initiative (CCSI) Toolset

FECM/NETL CO_2 Transport Cost Model

FE/NETL CO_2 Saline Storage Cost Model

FE/NETL CO_2 Prophet Model

FE/NETL Onshore CO_2 EOR Cost Model

FECM/NETL Unconventional Shale Well Economic Model

Life Cycle Analysis Models

NETL CO2U LCA Guidance Toolkit

NETL UPGrants LCA Guidance Toolkit

IDAES Integrated Platform

IDAES Power Generation Model Library

Pulverized Coal Carbon Capture Retrofit Database (CCRD)

Natural Gas Combined Cycle CCRD

Industrial Sources CCRD

Key Reports

Baseline Studies for Fossil Energy Plants

Cost of Capturing CO_2 from Industrial Sources

Quality Guidelines for Energy System Studies

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