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.
RL for Adaptive Control of Flexible Plant Operations
Discussed in Paper

A novel application of reinforcement learning (RL) for online dynamic tuning of model predictive controllers (MPC) was described in a paper co-authored by SSAE researchers Stephen Zitney and Benjamin Omell and researchers from the Department of Chemical and Biomedical Engineering at West Virginia University. The proposed RL approach uses temporal difference learning with a control-specific reward function to improve the error tracking performance of the MPC formulation. The RL-MPC algorithm was applied to a case study of controlling nitrogen oxide (NOx) emissions in an industrial selective catalytic reduction (SCR) unit. Along with an RL-MPC formulation for NOx control, another MPC was developed to mitigate ammonia slip and decrease ammonia consumption in the SCR during load-following operation. Published in the *Computers & Chemical Engineering* journal, the study demonstrated the promise of online application of RL-MPC not only for systems where optimal MPC tuning parameters change with time and/or servo control and/or disturbance rejection tasks, but also for systems where it is hard to obtain optimal tuning parameters in general without significant trial-and-error that may not be acceptable to plant personnel.

Kinetic Model Development Discussed in Recent Paper

Development of kinetic models for reduction of an iron-based oxygen carrier particle with methane, carbon monoxide and hydrogen was discussed in a paper by Anca Ostace* et al.

The Bayesian model-building and uncertainty quantification framework presented in the paper, published in the *Chemical Engineering Science* journal, enables the simultaneous quantification of parameter and model form uncertainty and was applied to develop the kinetic models. The developed models show excellent agreement between model predictions and both calibration and validation data. Parameter uncertainty is quantified by determining their joint posterior distribution, and model structure uncertainty is accounted for by incorporating stochastic discrepancy functions into basis mechanistic kinetic models. The hybrid kinetic models with discrepancy functions are suitable for use in both stochastic and deterministic studies in equation-oriented modeling and optimization platforms like the Institute for the Design of Advanced Energy Systems (IDAES).

New SOC Cost Modeling Tool Debuts

SSAE recently released a robust and flexible Solid Oxide Cell (SOC) and Stack Manufacturing Cost Tool capable of estimating production costs of solid oxide fuel cells and electrolysis cells with different geometries. The analysis tool will assist commercial developers and researchers in evaluating the costs of manufacturing large volumes of SOCs and stacks, aiding the development and commercialization of SOC technology.

The toolset breaks factors down between materials, labor, utilities, capital and indirect costs to generate a total annual cost, cost per stack and cost per kilowatt (kW) (or cost per kilograms hydrogen) based on user inputs for capacity. The Excel-based tool features a user-friendly workflow to update default values between tabs. It is also capable of performing sensitivity analysis on various input parameters to demonstrate the effect on total costs. Within the tool, advanced users can add custom materials and manufacturing methods or create another SOC design. Learn more.

Stack Cost Component Breakdown

The example breakdown of SOC stack costs provided by the tool ($/kW) is as follows:

- **Material**: $22.16, 9%
- **Labor**: $33.35, 13%
- **Utilities**: $31.37, 13%
- **Capital**: $26.05, 10%
- **Indirect**: $135.45, 55%

Total Stack Cost: $248.39 /kW

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*NETL Support Contractor*
New Version of the CO2_T_COM Released

A new version of one of SSAE’s open-source carbon capture, utilization and storage (CCUS) models was recently released. Developed by the U.S. DOE’s Office of Fossil Energy and Carbon Management (FECM)’s NETL, the FECM/NETL CO₂ Transport Cost Model (also known as CO2_T_COM) is an Excel-based tool that estimates revenues and capital, operating and financing costs and calculates the break-even cost (in $/tonne) for transporting liquid phase carbon dioxide (CO₂) by pipeline. With its flexible interface, users can tailor the model to fit their project requirements. A user’s manual and overview presentation were also released. Learn more.

Since its last release in May 2018, several updates have been made to the model including adding the ability to calculate costs in real dollars, changing the CO₂ equation of state, adding several macro options to calculate costs, correcting errors for elevation change along the pipeline and revising the algorithm for determining the number of booster pumps and associated nominal pipe size that give the lowest first-year break-even CO₂ price.

As the U.S. moves toward decarbonization, management strategies (e.g., expanding CCUS) will be at the forefront. The CO2_T_COM can help evaluate integrated CCUS networks (i.e., connecting a CO₂ source to a storage site) and costs of large-diameter trunklines or shorter, smaller pipelines (e.g., gathering/distribution).

SSAE Reports Respond to Executive Order on Key Energy Technology Supply Chains

The U.S. DOE released a report in February 2022 on challenges and opportunities met by the U.S. energy supply chains and federal government plans to address these items. In response to Executive Order 14017 “America’s Supply Chains,” several deep dive assessments on various clean energy technologies were issued supplementary to this report including those that involved SSAE researchers. The White House and the Presidential Administration will utilize these reports to inform decisions, develop policy and strategy and ultimately help the United States mitigate their environmental footprint over the coming decades in the most effective and efficient manner possible.

- “Carbon Capture, Transport, & Storage – Supply Chain Deep Dive Assessment” reviewed material and component requirements that may be necessary to ramp up carbon capture and storage (CCS) to 2 gigatonnes per annum (Gt/yr) of CO₂ by 2050 and evaluated what supply chain challenges and opportunities this may create. For this assessment, monoethanolamine (MEA)-based CO₂ capture systems were assumed, with 96,694 miles of pipeline infrastructure connecting to a network of 2,938 storage wells across the United States capable of handling 2 Gt/yr by 2050. The study found that most of the materials required for this undertaking could readily be obtained given existing production, with peak annual triethylene glycol (TEG) and steel pipe required hitting 40.6 kilotonnes (Kt) (8.1% of current global production) and 6.5 megatonnes (10.6% of current global production), respectively (see chart below). MEA annual estimates top out at 834 Kt (45.3% of current global production) in 2050, demanding a prudent yet feasible increase in manufacturing (10-15% compound annual growth rate) in the coming decades. All other material requirements were considered negligible. Building out this CCS network would benefit the climate and create growth in the U.S. economy and workforce.

- “Water Electrolyzers and Fuel Cells Supply Chain - Supply Chain Deep Dive Assessment” examined potential supply chain and materials issues and opportunities for electrolyzers and fuel cells in a decarbonized future to meet a 100 million metric tonnes per year electrolytic hydrogen market. The SOC and Stack Manufacturing Cost Tool was used to calculate critical materials information for SOC technology. The assessment found that for this market to grow to this size, the electrolyzer capacity required ranges up to 1,000 gigawatts (GW), which results in an approximately 20% compound annual growth rate from 2021 to 2050. Additionally, over 50 GW of domestic fuel cell capacity is required with an annual manufacturing requirement of over 3 GW/yr. The study also found that there would be an increased need for domestic extraction and refining of many key materials since they are currently primarily (and exclusively, for some) imported.
HIGHLIGHTS (cont’d)

NETL-SSAE to Lead Tri-Lab IES Analysis Effort

NETL-SSAE will lead a Tri-Lab Integrated Energy Systems (IES) Analysis with the National Renewable Energy Laboratory (NREL) and Idaho National Laboratory (INL) to support PNW Hydrogen LLC in a recently awarded project to produce clean hydrogen from nuclear power at the Palo Verde Generating Station in Phoenix, Arizona. The project will receive $12 million from DOE’s Hydrogen and Fuel Cell Technologies Office (HFTO) and $8 million from DOE’s Office of Nuclear Energy. Six tonnes of stored hydrogen will be used to produce approximately 200 megawatt hours of electricity during times of high demand and may also be used to make chemicals and other fuels. The project will provide insights about integrating nuclear energy with hydrogen production technologies and inform future clean hydrogen production deployments at scale.

The NETL-led team will collaborate on a joint analysis of the Arizona Public Service (APS) regional bulk power system to quantify the benefits of hydrogen production as a vector to secure the future of the Palo Verde Generating Station and to assess opportunities for a broader build-out of hydrogen generation and use. This will support APS in achieving its goal of reaching 100% clean power by 2050. The Tri-Lab Analysis Team will leverage the Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems (DISPATCHES) developed under DOE’s Grid Modernization Laboratory Consortium (GMLC) by NETL, Sandia National Laboratories (SNL), Lawrence Berkeley National Laboratory (LBNL), NREL and INL.

PNW Hydrogen LLC will be the primary recipient of the DOE award and will collaborate with multiple stakeholders in research, academia, industry and state-level government including NETL, INL, NREL, OxEon, Electric Power Research Institute, Arizona State University, University of California Irvine, Siemens, Xcel Energy, Energy Harbor and the Los Angeles Department of Water and Power.

Staff Spotlight

Since joining the Life Cycle Analysis (LCA) Team last September, Gabby Yanai* advanced work under the Oil and Gas Program, Coal Beneficiation Program and CO2 Utilization LCA Support. She researched and calculated the potential global warming effects of blending hydrogen and renewable natural gas into the fossil natural gas pipeline which is part of a larger investigation into natural gas as a decarbonization strategy; helped assess the environmental performance of various carbon-based synthetic graphite production processes and provided technical reviews of LCA related to CO2 utilization technologies and products.

Yanai graduated from Carnegie Mellon University (CMU) with a B.S. in Chemical Engineering, an additional major in Engineering and Public Policy and a minor in Professional Writing. She spent the last two years at Kia Motors in their Inclusion & Diversity Department and interned at NASA’s Jet Propulsion Laboratory and The National Academies of Sciences, Engineering and Medicine. Originally from Los Angeles, California, Yanai enjoys reading and playing basketball and was a member of the women’s basketball team while at CMU.

NOTICES

SSAE Collaborators Receive Honors

Two key SSAE collaborators who are part of IDAES and contributed significantly to the Carbon Capture Simulation Initiative (CCSI), recently received honors for their work:

- Nikolaos Sahinidis (Georgia Tech) was elected to the National Academy of Engineering (NAE) for his “contributions to global optimization and the development of widely used software for optimization and machine learning (ML).” NAE election is among the highest recognitions awarded to engineers for accomplishments in engineering research, practice, education, literature and technology. Sahinidis developed BARON, global optimization software that solves challenging mathematical optimization problems, and ALAMO, the only tool that can impose physical constraints on ML models and generate interpretable models from the fewest possible data. Sahinidis will be formally inducted at the NAE’s annual meeting in October 2022.

- Lorenz Biegler (CMU) won the Sargent Medal of the Institution of Chemical Engineers for his impact on theory, algorithms, software and chemical engineering applications in the optimization of process systems. This medal recognizes contributions to computer-aided product and process engineering research.
SSAE Researchers Receive Best Paper Award
Sandeep Pidaparti*, Charles White* and Nathan Weiland received a Best Paper plaque for “A Performance and Economic Comparison of Partial Cooling and Recompression sCO2 Cycles for Coal-Fueled Power Generation” at the 7th International Supercritical Carbon Dioxide (sCO2) Power Cycles Symposium in February 2022. This study highlighted the importance of focusing research and development (R&D) on the primary heater, the main contributor to plant cost, sCO2 cycle pressure drop and cost of electricity (COE).

For this study, techno-economic analyses were conducted to compare the performance and COE of recompression and partial cooling cycles for coal-fired power plants. A simplified circulating fluidized bed (CFB) design tool was developed to explore the impact of design variables on CO2 pressure drop and CFB cost. Results showed that the partial cooling cycle yields lower recuperation and CFB costs relative to recompression cycles. Thus, partial cooling cycles also resulted in a lower COE than recompression cycles.

LCA Work Featured at Various Conferences
SSAE researchers presented LCA work at several virtual conferences in 2022:

- Life cycle greenhouse gas analysis of direct air capture (DAC) systems was featured in a presentation by Matthew Jamieson et al. at a session focusing on key takeaways from recent DAC LCAs at the United States Energy Association DOE-FECM DAC LCA Workshop in January 2022.
- An overview of NETL’s upstream natural gas LCA modeling was presented by Timothy Skone at the Methane Characterization in Electric Utility Natural Gas Systems: Electric Power Research Institute’s Winter 2022 Advisory Meeting in February 2022.
- LCA tools to evaluate the environmental footprint of carbon utilization projects was highlighted in a presentation by Sheikh Moni* et al. at the Indo-U.S. Scoping Workshop on Carbon Utilization and Conversion in February 2022. The goal of this workshop was to identify capabilities within each country on carbon utilization/conversion technologies, common R&D technical challenges and opportunities.

H₂ Production Pathways Discussed at Workshop
The status of the upcoming “Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies” study along with an overview of NETL analysis efforts to support the DOE Hydrogen Shot targets was presented by Eric Lewis at the 2022 Bulk Storage of Gaseous Hydrogen Workshop, which was sponsored by DOE’s HFTO and held in February 2022. The study analyzes plant performance, life cycle environmental performance and the levelized cost of hydrogen production from six fossil-based pathways. Preliminary results pending finalization of this study, which is anticipated to be in the March–April 2022 time frame, were also provided in this presentation.

Future of “Project PARETO” Discussed at Stakeholder Meeting
As part of DOE’s produced water optimization initiative, SSAE’s Markus Drouven conducted the first quarterly “Project PARETO” Stakeholder Board Review Meeting of 2022. The initiative is developing an optimization-based decision-support software framework, PARETO, that will help organizations better manage, treat and beneficially reuse produced water. The stakeholder meeting included more than 50 attendees representing the produced water community in its entirety (i.e., upstream operators, midstream companies, technology providers, consultants, etc.). In addition to updating the Board on project accomplishments, the meeting involved three parallel breakout sessions on topics of interest, including: 1) recovering critical minerals/rare earth elements from produced water, 2) carbon storage opportunities for the produced water community, and 3) regulatory solutions for beneficial reuse of produced water. Seventy percent of participants confirmed that they expected their organization to make use of DOE’s PARETO software in the near future, and 30% selected “maybe”. The stakeholder meeting allowed the project team to collect specific feedback on how PARETO can be further refined and deployed most effectively. “Project PARETO” is funded by FECM’s Advanced Remediation Technologies Program.

SSAE CORE CAPABILITIES

Process Systems Engineering at NETL
Process systems engineering (PSE) brings together domain expertise in engineering, operations research, statistics and applied mathematics to support decision making for the design and operation of processes and systems for various products, including electricity and hydrogen. These processes and systems are becoming increasingly dynamic and interconnected, requiring new capabilities to effectively understand design and operating options. Decision-making tools now need to extend beyond traditional plant boundaries and consider interactions with broader supply chains, including the electricity grid and pipelines.
SSAE’s PSE team focuses on developing and applying advanced, state-of-the-art computational approaches to address questions beyond the reach of traditional commercial techniques. These applications typically rely on rigorous mathematical optimization of detailed physics-based models to understand new opportunities for optimizing the design and operation of complex, dynamic, interacting energy and industrial systems to increase efficiency, lower costs, increase revenue, improve sustainability and facilitate deep decarbonization. Applications range from supporting decarbonization of the U.S. power industry to developing the U.S. energy, water and manufacturing systems of the future.

The PSE team leads the development and application of these advanced capabilities in collaboration with researchers from multiple national laboratories and universities, resulting in open-source capabilities widely available for industry and other researchers to use and extend. In addition, industrial participants are actively engaged as stakeholders through monthly meetings, annual workshops, training webinars and collaborative projects.

Carbon Capture Simulation for Industry Impact (CCSI2) combines the Framework for Optimization and Quantification of Uncertainty (FOQUS) with predictive, first-principles models often developed in commercial software, such as Aspen Plus®, Aspen Plus Dynamics™ and Aspen Custom Modeler®, to maximize the learning from laboratory and pilot-scale testing and reduce technical scale-up risk through rigorous optimization, uncertainty quantification (UQ) and statistical design of experiments. The scientific underpinnings pioneered during CCSI and encoded into the suite of models ensures that learning is maximized through development of successive technology generations. CCSI2 collaborators include LBNL, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory (ORNL), West Virginia University (WVU), University of Toledo and University of Pittsburgh.

IDAES builds on the success of CCSI, enabling more extensive optimization and intrusive UQ of larger, more complex systems through a fully open-source integrated platform that combines the capabilities of state-of-the-art process simulation packages and general algebraic modeling languages (AML). This enables IDAES to address emerging challenges and opportunities in the energy and process sectors that cannot be addressed by current tools. These include the need to design and optimize processes that are more tightly coupled with external systems and incorporate new technologies with inherently dynamic operation such as IES. IDAES is built on Pyomo, a Python®-based AML designed specifically to address challenges in formulating, manipulating and solving large complex structured optimization problems. The platform empowers users to create models of novel processes and rapidly develop custom analyses, workflows and end-user applications. Collaborators include SNL, LBNL, CMU, WVU, University of Notre Dame and Georgia Tech.

The open-source CCSI Computational Toolset and IDAES Integrated Platform each received R&D 100 awards for their pioneering capabilities including, but not limited to:

- Predictive physics-based modeling: efficient workflows for data reconciliation, parameter estimation and model validation for innovative, new processes and materials that enable identification of data gaps and potential pitfalls.
- Process synthesis and conceptual design: reliable and efficient construction and optimization of superstructures of process alternatives to identify novel configurations and opportunities for process intensification.
- Process design and optimization: large-scale, system-wide optimization of process equipment and operating conditions (e.g., temperatures, pressures, flow rates, compositions) using rigorous models that maintain accuracy across broad ranges of operation.
- Multi-scale surrogate modeling: inference and training of ML models as surrogates for more complex first-principles, data-driven or hybrid models to increase the size and complexity of multi-scale systems that can be optimized.

Additional core capabilities developed specifically for technical risk reduction include:

- Uncertainty quantification: understanding how various forms of uncertainty (e.g., operational, economic, epistemic) may interact and impact key performance indicators.
- Robust optimization: development of “robust” process designs that guarantee required performance in the face of known uncertainties at minimal cost.
- Sequential design of experiments: optimal design of test campaigns that generate data aimed at minimizing process uncertainties thereby reducing future scale-up risk.

These capabilities are currently being applied in several application areas including design and optimization of carbon capture systems, CO₂ removal, solid oxide fuel cells and electrolyzer cells and energy storage, as well as hydrogen production and utilization. The IDAES Integrated Platform also serves as the core modeling framework for two additional multi-institutional collaborations:

- **Design Integration and Synthesis Platform to Advanced Tightly Coupled Hybrid Energy Systems (DISPATCHES)**, which is part of the DOE GMLC, supports the design, optimization and analysis of tightly coupled IES within the bulk power system via market signals. Collaborators include SNL, LBNL, INL, NREL and University of Notre Dame.
- **WaterTAP**, funded through the Advanced Manufacturing Office’s National Alliance for Water Innovation (NAWI) Desalination Hub, is creating model libraries to enable techno-economic assessments of water treatment processes systems as well as their design and optimization. Collaborators include LBNL, NREL and ORNL.
The PSE team also possesses deep expertise in dynamic process modeling to explore control and operational feasibility as well as digital twins to enable evaluation of control and operation schemes for a broad range of transient conditions including process start-ups, shutdowns, upsets, malfunctions and other disturbances. Such capabilities enable the development of processes that can meet the requirements of a broad range of future energy scenarios while minimizing the negative impacts to efficiency, emissions and component health.

Most recently, the PSE team kicked off “Project PARETO” to develop an open-source, optimization-based, produced water decision support application in support of DOE’s Produced Water Optimization Initiative. Specifically, the platform will support coordination of produced water deliveries, buildout of the produced water infrastructure in terms of pipelines and storage facilities, the selection of effective treatment technologies, the placement and sizing of treatment facilities, the identification of beneficial water reuse options and the distribution of treated produced water and/or concentrated brine for beneficial reuse. – Contributed by Anthony Burgard, SSAE’s Process Systems Engineering Research Team and David Miller, SSAE’s Senior Fellow.

SSAE Federal staff and NETL support contractor personnel will attend or present at the following conferences and events in April 2022:

• North American Electric Reliability Corporation Reliability Assessment Subcommittee Spring Meeting
  Participant: John Brewer
  Virtual, April 13–14, 2022

• Appalachian Hydrogen & Carbon Capture Conference
  Participant: Justin Adder
  Hybrid (Virtual and Canonsburg, PA), April 21, 2022

• 2022 Society of Petroleum Engineers (SPE) Western Regional Meeting
  Presenter: Nur Wijaya*
  Bakersfield, CA, April 26–28, 2022

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2022 SPE Western Regional Meeting
Bakersfield, CA, April 26–28, 2022

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// RECENT PUBLICATIONS

Manuscripts


Model/Tool


Reports/Supporting Documentation

- **K. Bello**, **D. Vikara**, **D. Morgan** and **D. Remson**, **“Dimensionally Reduced Model for Rapid and Accurate Prediction of Gas Saturation, Pressure, and Brine Production in a CO₂ Storage Application: Case Study Using the SACROC Field as Part of Smart Task 5,”** National Energy Technology Laboratory, Pittsburgh, PA, March 2022.


Presentation


Conference Proceedings and Events


Models / Tools / Databases
- FECM/NETL CO₂ Transport Cost Model
- FE/NETL CO₂ Storage Cost Model
- FE/NETL CO₂ Prophet Model
- FE/NETL Onshore CO₂ EOR Cost Model
- Life Cycle Analysis Models
- NETL LCA CO₂U toolkit
- 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
- Quality Guidelines for Energy System Studies
- Life Cycle Analysis

SSAE website
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- Life Cycle Analysis webpage
- CCSI2 webpage

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