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.

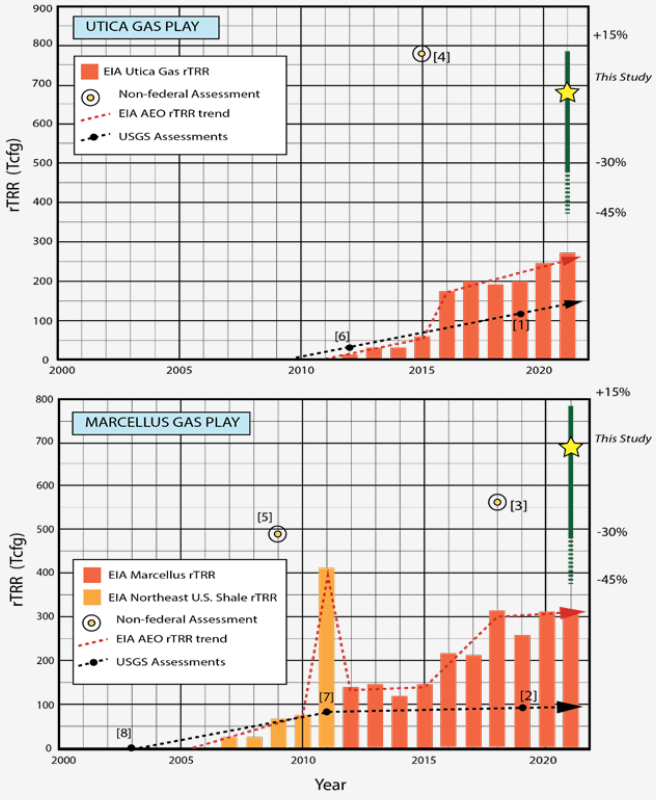
// HIGHLIGHTS

Assessment Supports Substantial Appalachian Shale Gas Resources

A newly released manuscript, "New assessment suggests substantial Appalachian shale gas resources," co-authored by **Ray Boswell** was featured in the November 2021 issue of the *Oil & Gas Journal*. This data-driven study used a new approach to estimate technically recoverable gas resources in the Marcellus and Utica shale plays.

The study estimated 693 trillion cubic feet (tcf) remaining (undiscovered) technically recoverable gas resources for the Marcellus play and 684 tcf for the Utica gas play. Both values exceed many recent estimates.

Despite a decade of extensive development, there is increasing uncertainty in assessing remaining resource potential of Appalachian basin shale gas plays. This study addresses these uncertainties and summarizes SSAE's new approaches to resource assessment.



SSAE Demonstrates Advanced Water Treatment Modeling Capabilities

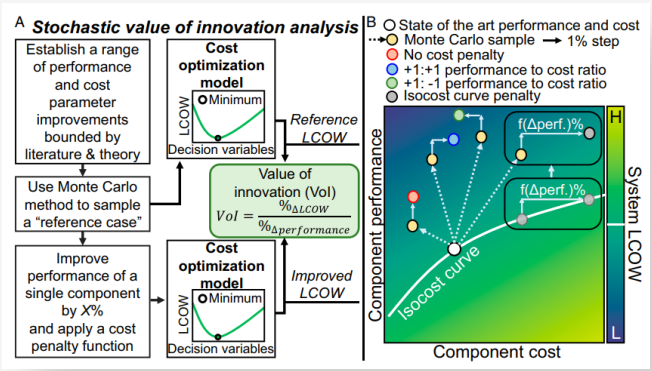
As part of the National Alliance for Water Innovation (NAWI) efforts to advance early-stage water treatment technologies, SSAE has led the development of ProteusLib, a water treatment model library compatible with NETL's Institute for the Design of Advanced Energy Systems (IDAES) platform. After one year of development, the model library was able to demonstrate:

- The first techno-economic assessment (TEA) of a low salt rejection reverse osmosis (RO) system. SSAE researchers minimized the levelized cost of water across its full application space.
- A TEA of a high-pressure RO treatment train which included pre-treatment and post-treatment processes and explicitly constrained the system to prevent gypsum mineral scaling.
- A digital twin of a commercial seawater desalination plant that accounts for 90% of the plant energy consumption. The digital twin was developed from plant operating data.

SSAE Researcher Co-authors Paper on Emerging Membranes for Desalination

Research proposing an analysis to identify the most impactful improvements for a process by quantifying a new metric ("value of innovation") was discussed in a paper co-authored by SSAE researcher **Tim Bartholomew**. This study, "High-impact innovations for high-salinity membrane desalination," was published in September 2021 in the Membrane Separations Science Special Feature of the *Proceedings of the National Academy of Sciences*.

This metric quantifies the impact on an outcome (e.g., the levelized cost of water) from improving the performance of a component by a percentile in a defined feasible range. The analysis uses advanced process systems engineering methods, including an equation-oriented cost optimization model and stochastic sampling, to determine a distribution of the value of innovation for multiple components while considering the uncertainty in simultaneous performance improvements.



// HIGHLIGHTS cont'd

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

NETL is leading a collaboration with several national laboratories and utility partners to develop DISPATCHES, a first-of-its kind computational platform to support the design, optimization and analysis of tightly coupled hybrid energy systems within the bulk power system via market signals. The capabilities developed as part of this effort can be used to help support NETL's mission, particularly the design of integrated energy systems incorporating market interactions with the bulk power system.

This three-year project, part of the Grid Modernization Lab Consortium, will specifically use three candidate energy systems (fossil + CCS + thermal storage + hydrogen, nuclear + hydrogen and renewables + storage + hydrogen) as case studies to establish an open-source platform and mathematical formulation for the design of hybrid systems.

The team is focusing on publishing manuscripts on the optimization approach and identifying designs for the three case studies. Efforts are also underway to collaborate with Exelon and the National Rural Electric Cooperative Association (NRECA) on some case studies.

NETL Moves Forward with FLExible Carbon Capture and Storage (FLECCS)

In two separate projects awarded under Advanced Research Projects Agency-Energy's (ARPA-E) FLECCS program, NETL is collaborating with multiple technology and utility partners to evaluate CCS technologies that enable power generators to be responsive to grid conditions in a high variable renewable energy (VRE) penetration environment. The program's primary goal is to design flexible capture systems that maximize the net present value (NPV) for a power generator operating in a high VRE grid with carbon prices of $100 to $300 per ton. This research will help accelerate development of flexible carbon capture technologies, which will be a critical component for a decarbonized grid.

In the first project, NETL will contribute to the evaluation of a rapid cycle thermal swing adsorption CO_2 capture technology. Earning the highest-ranked GREEN technical status on all tasks by ARPA-E, the project's workflow, enabled by IDAES, entails formulating and solving an NPV maximization problem that identifies the optimal flexible capture system design for a given market assuming a price-taker approach (i.e., the designed plant will not impact electricity market prices). The team is currently working on incorporating different costs based on inputs from the industrial partners to accurately compute the NPV in the optimization problem.

In the second project, NETL will collaborate with RTI International to develop a cost-effective, resilient, load-following, intensified rotating packed bed centrifugal absorber design using advanced water-lean solvents and novel solvent regeneration strategies for decarbonizing natural gas power plants. Enabled by CCSI^2, the project team will develop simulations of the novel process design, validated by bench scale data, which will be used to maximize the NPV of the of low carbon electricity sales under dynamic plant loads and high VRE environments.

Both NETL FLECCS projects are currently in Phase 1, which is focused on design and analysis to computationally evaluate the potential for these novel technologies to contribute to decarbonization of a VRE grid. Phase 1 will be followed by pilot-scale demonstrations if the projects are selected to proceed to Phase 2.

// NOTICES

Shultz in the Spotlight at LEAP Workshop

NETL analyses supporting low-carbon emissions and/or carbon-negative energy generation were highlighted by **Travis Shultz** at the 6th Low Emission Advanced Power (LEAP) Workshop held November 1–4, 2021. Shultz's presentation was given during a panel discussion on transition cost and impact.

The workshop focused on supporting the building of a carbon pollution-free electricity sector by 2035 and the need to advance development of innovative technologies in this decade to decarbonize the U.S. power sector.

// NOTICES cont'd

SSAE Researchers Present at EMRE/National Lab Joint R&D Meeting

Over the last two years, ExxonMobil Research & Engineering Company (EMRE) has worked in partnership with the National Renewable Energy Laboratory (NREL), NETL and other national laboratories to create a portfolio of programs to address key challenge areas associated with the future of energy.

The partners held a joint meeting November 2–3, 2021 to discuss four thematic areas (hydrocarbon processing efficiency, power and the grid, biomass conversion and carbon management). **Travis Shultz** and EMRE and NREL researchers discussed the future of the power grid, while **Jaffer Ghouse*** and an EMRE researcher discussed the direct air capture process landscape.

Tarka Part of Team That Earns R&D 100 Award

Tom Tarka, along with other NETL researchers, earned a prestigious R&D 100 Award for the development of a game-changing suite of low-cost, versatile sorbents that is highly effective in cleaning contaminated waterways and removing metals from electronic and pharmaceutical production processes.

Their innovation, known as Multi-functional Sorbent Technology, offers a practical, affordable and green approach to recover critical materials (e.g., aluminum and cobalt) and removes the threat of selenium, lead and other heavy metals that contaminate water supplies

The R&D 100 Awards competition annually recognizes 100 winning products and technologies as the disruptors that will change industries and make the world a better place in the coming years.

NETL Advances REE Production in Wyoming

NETL's Research & Innovation Center (RIC) has been working extensively with academic and industrial partners in Wyoming for several years to evaluate the resource potential for critical mineral (CM)/rare earth element (REE) production in the state.

Research has included the collection and analysis of core samples (sampling campaigns), which has led to the discovery of REE "hot spots" within Wyoming coal seams (e.g., areas within a coal seam with elevated concentrations of REEs) and the validation of NETL's Unconventional Rare Earth Element and Critical Mineral (URC) model. This model is designed to locate promising unconventional deposits of REEs. It also includes a Technology Commercialization Fund (TCF) award to demonstrate the production of REEs from Powder River Basin (PRB) coal ash at the pilot scale in Gillette, Wyoming, using an NETL-developed technology.

SSAE's **Tom Tarka**, a co-PI on the TCF project and the portfolio lead of RIC's Critical Minerals Field Work Proposal (FWP), presented to Wyoming stakeholders the potential for REE recovery from the state's resources as part of a webinar on November 15, 2021. The presentation provided an overview of NETL's research into REE recovery from unconventional CM/REE resources (e.g., coal and coal ash), as well as the opportunities and challenges of these resources.

Congratulations to Researchers on the SSAE-Led Critical Minerals FWP Team

SSAE's **Tom Tarka** leads NETL-RIC's Critical Minerals FWP which includes efforts of the Critical Minerals FWP Team. This work portfolio investigates how to unlock the potential of the U.S. domestic, unconventional REE/CM resources. Within the last two years, three researchers from this team, (**Mengling Stuckman***, **Jinichiro Nakano*** and **Fan Shi***) have been distinguished as Leidos Technical Fellows in part for their roles on this effort. Leidos is an approximately 40,000-person Fortune 500 company; these researchers join a list of 100 employees recognized as Technical Fellows

SSAE Research Highlighted at AIChE Annual Meeting

SSAE researchers and work products were well represented at the American Institute of Chemical Engineers (AIChE) Annual Meeting held November 7–19, 2021:

- An overview on NETL's CO_2 Utilization Life Cycle Analysis (LCA) Toolkit, its utility to the LCA community and its value in assessing emerging technologies was discussed in a presentation co-authored by **Sheikh M. Moni***, **Matthew Jamieson** and **Timothy Skone**.
- Research on advanced machine learning-augmented model predictive control, equipment health modeling and dynamic optimization of flexible power plant operations was highlighted in several presentations co-authored by **Steve Zitney** and **Ben Omell**.
- The application of the IDAES Integrated Platform to multi-scale optimization of market interactions, conceptual design of energy storage systems and flexible operation of amine-based carbon capture was highlighted in presentations co-authored by **Jaffer Ghouse***, **Miguel Zamarripa***, **John Eslick*** and **David Miller**.
- Use of CCSI² tools to optimally design an monoethanolamine-based carbon capture system for the cement industry as well as design, optimize and control microencapsulated solvent-based carbon capture systems was highlighted in presentations co-authored by **Daison Caballero***, **Miguel Zamarripa***, **Ben Omell** and **Mike Matuszewski***.
- A session on design and optimization of integrated energy systems was chaired by **David Miller**.

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// PERSPECTIVES

IHS Coal Briefing

On October 19, 2021, NETL SSAE staff was briefed by IHS on both domestic and international coal markets. A summary of key takeaways from the briefing:

U.S. Coal:

- There is a general lack of investment in coal mines, but this problem is not unique to the U.S.
- Overall U.S. production was up in 2021 Q3 mostly from increases in PRB production.
- The U.S. is starting at a low base on stockpiles and will likely see days of burn fall below 50 days this winter.
- The only real price advantage over gas currently for coal in the U.S. is PRB into the Electric Reliability Council of Texas.
- Most metric tons in the United States are contracted, rather than spot purchased.
- IHS anticipates U.S. coal-fired power plant (CFPP) retirements will accelerate in 2022 and 2023. This is projected to result in the overall capacity factor of the domestic CFPP fleet to increase from 44 percent today to 56 percent in 2024.

International Metallurgical Coal:

- Seaborne metallurgical coal trade in 2021 is projected to be higher than 2020 levels, but lower than 2019. India is the country with the projected largest increase in year-over-year imports in 2021.
- Prices have been at very high levels, with seaborne spot coal prices having quadrupled over prices a year ago. China's imports are the key driver contributing to high prices, as China is exhibiting strong demand while currently not importing coal from Australia (its traditional leading supplier, often accounting for half of China's metallurgical imports).
- During the first half of 2021, the leading suppliers of China's metallurgical coal imports were Mongolia (8.8 million metric tons), Russia (5.6 million metric tons), Canada (4.8 million metric tons) and the U.S. (4.5 million metric tons). This is a stark change from 2020 when Australia supplied about 50% of China's metallurgical coal imports.
- IHS projects growth in the global trade market through 2030 with India leading the increase in demand. From 2030-50, it projects the seaborne metallurgical market will level out in terms of tonnage. Factors potentially limiting growth in coming years include a transition to electric arc furnace steel production (which is not directly reliant on metallurgical coal), underinvestment in the industry and environmental, social and governance concerns.

International Thermal Coal:

- Seaborne thermal trade in 2021 is projected to be higher than 2020 levels, but lower than 2019. China is the country with the projected largest increase in year-over-year imports in 2021.
- Some seaborne thermal prices are at price levels four times what they were a year ago. Demand is currently very strong relative to 2020 due to latent catchup demand from industries (e.g., fertilizer and cement), as well as restocking demand (low inventories) and underlying demand. Once latent catchup demand and restocking demand go away, thermal coal demand will be less than in 2019.
- Due to trade restrictions with China, Australia has shifted its exports increasingly to India, South Korea and Taiwan.
- IHS projects global thermal coal import demand will remain relatively flat until about 2030 and will subsequently decline. The main driver behind this decline is China's anticipated decrease in thermal coal imports which appears to be driven largely by China's pledge of obtaining carbon neutrality by 2060. China is the first country to make such a pledge where energy demand is still growing, and it anticipates there will be heavy investment in carbon capture, utilization and storage, but still anticipates China's coal demand will be largely curtailed. – Contributed by **Gavin Pickenpaugh**, SSAE's Energy Markets Analysis Team

// UPCOMING

SSAE Federal personnel will attend the following meeting in December 2021:

35th Annual Economic Outlook Symposium
Peter Balash (participant)
Virtual, December 3, 2021

// CONFERENCES AND EVENTS

Federal Reserve Bank of Chicago, 35th Annual Economic Outlook Symposium
Virtual, December 3, 2021

// RECENT PUBLICATIONS

Manuscripts

A. Dudchenko, **T. Bartholomew** and M. Mauter, "High-impact innovations for high-salinity membrane desalination," Membrane Separations Science Special Feature of the *Proceedings of the National Academy of Sciences*, vol. 118, no. 37, September 2021.

B. Carney, **R. Boswell** and S. Pool, "New assessment suggests substantial Appalachian shale gas resources," *Oil & Gas Journal*, November 1, 2021.

Conference Proceedings and Events

T. Shultz, "Overview of NETL Analyses Supporting Low Carbon Emissions and/or Carbon-Negative Energy Generation" presentation at 6th Low Emission Advanced Power (LEAP) Workshop – Session 3: Transition Cost and Impact, Virtual, November 1, 2021.

S. Moni*, **M. Jamieson** and **T. Skone**, "Life Cycle Analysis Tools to Evaluate Environmental Footprint of Carbon Utilization Projects," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

E. Hedrick, K. Reynolds, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Development of Algorithms for Reinforcement Learning Augmented Model Predictive Control," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

E. Hedrick, K. Reynolds, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Nonlinear Predictive Control of an Industrial Selective Catalytic Reduction Unit with Time-Varying Time Delay," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

K. Reynolds, E. Hedrick, **B. Omell**, **S. Zitney** and D. Bhattacharyya, "Dynamic Optimization of the Operational Trajectory of a Supercritical Pulverized Coal-Fired Boiler Under Load-Following with Consideration of Boiler Health," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

K. Reynolds, E. Hedrick, **B. Omell**, **S. Zitney** and D. Bhattacharyya, "Health Monitoring of an Industrial Supercritical Pulverized Coal Boiler," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

E. Hedrick, K. Reynolds, S. Hong, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Advanced Model Predictive Control for Reducing Equipment Damage in a Supercritical Pulverized Coal Fired Power Plant during Load-Following Operation," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

G. Kotamreddy, R. Hughes, D. Bhattacharyya, **B. Omell** and **M. Matuszewski***, "Dynamic Modeling and Soft Sensor Based Predictive Control of a Moving Bed Process for CO_2 Capture Using a Micro-Encapsulated Solvent," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

G. Kotamreddy, R. Hughes, D. Bhattacharyya, **B. Omell** and **M. Matuszewski***, "Optimal Selection of Solvent and Contactor Technology for Micro-Encapsulated Carbon Sorbent (MECS) Based CO_2 Capture," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

L. Deng*, **D. Caballero***, **M. Zamarripa***, B. Kutchko, C. Tao, **B. Omell** and **M. Matuszewski***, "Design of an MEA-Based Carbon Capture System for Cement Industry," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

E. Rawlings, N. Susarla*, **J. Ghouse***, **M. Zamarripa***, C. Laird, J. Siirola, M. Bynum and **D. Miller**, "Conceptual Design Via Superstructure Optimization in Advanced Energy Systems Using IDAES," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

J. Jalving, **J. Ghouse***, B. Knueven, J. Siirola, A. Dowling and **D. Miller**, "Toward Future Energy Generation Systems: Multi-Scale Optimization with Market Interactions," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

P. Akula, **J. Eslick***, D. Bhattacharyya and **D. Miller**, "Rate-Based Dynamic Modeling and Optimization of an Amine-Based Carbon Capture Unit for Flexible Operation," presentation abstract for 2021 AIChE Annual Meeting, November 7-11 (Boston, MA) and 15-19 (virtual), 2021.

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// REFERENCE SECTION

Models / Tools / Databases

FE/NETL CO_2 Transport Cost Model

FE/NETL CO_2 Storage Cost Model

FE/NETL CO_2 Prophet Model

FE/NETL Onshore CO_2 EOR Cost Model

Life Cycle Analysis Models

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 Systems Studies

Life Cycle Analysis

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