NATIONAL ENERGY TECHNOLOGY LABORATORY

SSAE Newsletter

JUNE // 2023

VOLUME 3.4

// 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

Journal Paper Highlights Economic Tradeoffs for Unconventional Well

The economic tradeoffs of pressure drawdown management and the resulting gas production outlooks for a real, producing unconventional gas well in the Marcellus Shale of the Appalachian Basin was evaluated in a recent study by SSAE. Published in *Gas Science and Engineering*, the study used a techno-economic analysis approach coupled with physics-informed rapid predictive models and was developed under DOE's Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications Initiative Phase I, Task 7 efforts. The use of pressure maintenance in hydraulically fractured reservoirs via sustained production drawdowns can improve cumulative recovery and overall resource extraction efficiency compared to more rapid drawdown approaches aimed at generating high initial production. However, oil and gas operators typically pursue production strategies that maximize profitability over resource extraction efficiency due to the inherent variability of oil and natural gas markets. There is a lack of research comparing the economic viability and present value of unconventional wells produced under different strategies. This knowledge gap could spark operators' interest in altering their field development approaches.

Gas production forecast scenarios were generated using a novel physics-informed machine learning workflow and traditional reservoir simulation. The FECM/NETL Unconventional Shale Well Economic Cash Flow Model (UShWEM) was used to evaluate economic implications for different drawdown scenarios given specific reservoir characteristics, capital expenditures, operating expenses, taxes, royalties and market conditions. Statistical methods were used to evaluate the sensitivity of economic and production factors, such as timing and volume of gas production, prevailing economic and market conditions and overall estimated ultimate recovery on key profitability metrics (e.g., internal rate of return and net present value [NPV]), by analyzing 1,300 scenarios (see Figure 1) to identify statistical contrasts in the controlling features.

The results show that there is potential to maximize and improve unconventional well productivity using a slower pressure drawdown technique while still maintaining a profitable project. However, slower pressure drawdowns may delay the time for operators and investors to break even resulting in a lower present value for the project. Considerations of business and investment risks, such as the discount factor of the project's capital, can largely influence the potential present value of scenarios evaluated in the case study. As a result, there is a need for frequent evaluation of production strategies and project economics in near-real time as market dynamics evolve to optimize production operations. For more information on this study, please contact SSAE researchers Kolawole Bello*, Derek Vikara* or Luciane Cunha.

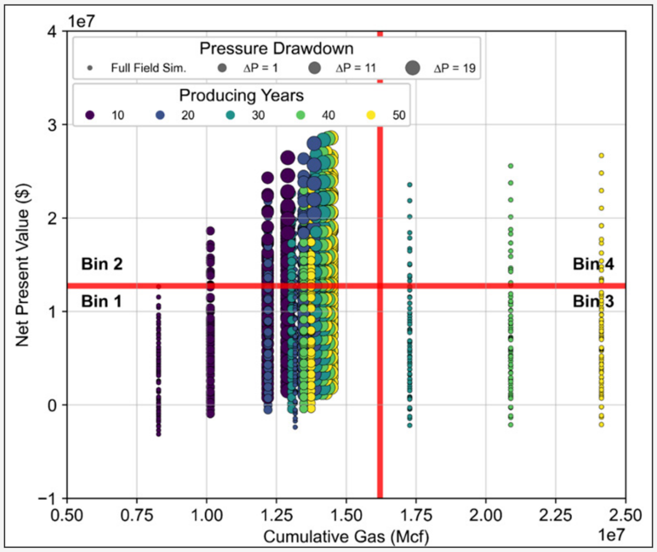

Figure 1. A quad chart highlighting the scenario placement across the spectrum of predicted output NPV and associated cumulative production. Scenario data is binned (1 through 4) for further analysis depending on where it falls in "high" or "low" groupings for NPV and cumulative production.

SCoRE Tool Highlighted in *Energy*

Replacing legacy high-carbon technologies with new low-carbon technologies, specifically those fueled by variable renewable resources (e.g., wind and solar), can disproportionally influence the costs associated with maintaining a reliable and competent grid system. A recently published paper in *Energy* detailed the results of a tool developed by SSAE researchers to estimate the system cost of replacement energy (SCoRE) —a metric for estimating how the total systems cost (TSC) might change in response to a technology replacement along the grid. The SCoRE tool was applied to nine replacement scenarios in the Electric Reliability Council of Texas operating region. Results highlight the carbon abatement targets able to be met by each of the new low-carbon technology options considered before changes in the TSC begin to increase exponentially.

Update to Low Rank Baseline Study Released

An independent assessment of the cost and performance of select fossil energy power systems —pulverized coal (PC), circulating fluidized bed and natural gas combined cycle (NGCC) plants at elevation— using a systematic, transparent technical and economic approach was presented in SSAE's recent release of the "Cost and Performance Baseline for Fossil Energy Plants Volume 3: Low Rank Coal and Natural Gas to Electricity." The cost and performance of fossil fuel-based generation technologies in the report are important inputs to assessments and determinations of technology combinations to be utilized to meet the projected demands of future power markets. The reference plant configurations provide perspective for regulators and policy makers. The report can be used to assess goals and metrics and provide a consistent basis for comparing developing technologies.

// HIGHLIGHTS cont'd

Technology Description	HHV Net Plant Efficiency (%)	Nameplate Capacity (MWe)	Cold Start (min)	Warm Start (min)	Hot Start (min)	Ramp Rate (%/min)	Minimum Load (%)
RICE – Spinning Mode (6x0)	41.3	113	N/A	10	5	60	9.7
RICE – Efficiency Mode (6x0)	41.3	113	N/A	10	5	23	0.8
RICE – Spinning Mode (12x0)	41.0	113	N/A	10	5	60	9.7
RICE – Efficiency Mode (12x0)	41.0	113	N/A	10	5	27	0.8
Aeroderivative NGSC (1x0)	38.8	116	N/A	10	8	43	16
Aeroderivative NGSC (2x)	36.0	105	N/A	10	5	95	50
F-Class Fast-Start NGCC (1x1)	52.8	375	130	50	35	11	49
H-Class Fast-Start NGCC (1x1)	54.8	560	130	85	30	11	38
F-Class Fast-Start NGCC (2x1)	52.9	751	120	45	32	11	50
F-Class Conventional-Start NGCC (2x1)	52.9	751	250	140	90	11	50
H-Class Fast-Start NGCC (2x1)	55.0	1,124	120	70	30	11	38

Figure 2. Flexibility metric results for RICE, aeroderivative CT and NGCC plants

New Baseline Study Released on Flexibility Attributes of Commercial Natural Gas Power Generation Technologies

The output of variable renewable energy (VRE) sources, such as wind and solar power generation, is intermittent, creating challenges to grid stability and reliability. Dispatchable fossil fueled generation is used to provide reliable power during periods of reduced VRE output. Dispatchable generators must be able to accommodate increasing VRE generation as the nation pursues the Administration's target of a decarbonized energy sector by 2035. As energy system experts create models (e.g., capacity expansion) to identify least-cost approaches to decarbonization, accurate cost and performance data characterizing dispatchable generators that operate flexibly at capacity factors that have been declining over time is needed to inform these models. Furthermore, these technologies continue to be a significant source of carbon dioxide (CO_2) emissions, providing the impetus for research and development (R&D), including the advancement and potential incorporation of carbon capture technologies.

To address the data needs of energy system modelers and to serve as a baseline for R&D, SSAE completed a study to characterize the flexibility attributes —both performance and cost — of nine common commercial natural gas-fueled electricity generating units. Although existing coal-fired power plants have served as baseload resources and have been increasingly relied upon as load-following resources, current natural gas technologies are much better equipped to follow intermittent renewable generation with faster ramping rates, shorter startup durations, higher efficiency, lower minimum loads, lower water usage, lower emissions and lower cost. The study, "Cost and Performance Baseline for Fossil Energy Plants, Volume 5: Natural Gas Electricity Generating Units for Flexible Operation," can provide valuable data as the nation pursues decarbonization.

The study included cases for reciprocating internal combustion engines (RICE), natural gas simple cycle (NGSC) aeroderivative combustion turbines (CT) and NGCC plants. While these cases do not include CO_2 capture, the data remains highly relevant given the ubiquitous current use of dispatchable, unabated natural gas power generation to back up VRE, and the results of some decarbonization modeling efforts that included the use of low-capacity factor unabated natural gas power generation well into the future. SSAE is also pursuing work to characterize the flexibility of power generation systems with integrated carbon capture. Figure 2 depicts the cases included in this study, as well as data for key flexibility metrics (learn more).

Rigorous Comparison of SOFC/SOEC-based Integrated Energy Systems Published

The cost and performance of several types of integrated energy systems based on solid oxide fuel cells (SOFC) to generate power and solid oxide electrolysis cells (SOEC) to produce hydrogen were evaluated in a recently published comprehensive technical report, "Technoeconomic Evaluation of Solid Oxide Fuel Cell Hydrogen-Electricity Co-Generation Concepts," by the Institute for the Design of Advanced Energy Systems (IDAES) researchers. All systems featured carbon capture rates exceeding 97%. Optimized process models were constructed using the IDAES® Integrated Platform and used to calculate overall production costs following a consistent methodology that facilitated comparisons of these process concepts to one another and to prior NETL cost and performance estimates. The analysis reveals that the best overall system is highly dependent on the assumed prices and demands of electricity and hydrogen because these determine the optimal mode of operation at a given point in time. Additionally, it suggests that integrated systems with the flexibility to produce either hydrogen or electricity can provide significant advantages over standalone systems that produce only hydrogen or only electricity in cases where future electricity prices are anticipated to be bimodal (e.g., distinct periods of low and high electricity prices) — a reasonable possibility in future high VRE grids.

Staff Spotlight

Since joining the Life Cycle Analysis (LCA) Team in May 2022, Roksana Mahmud* has developed biomass models and contributed to an associated screening tool, created a database of critical minerals studies, conducted critical reviews of rare earth extraction LCA reports and characterized feedstocks and pathways for gasification.

Roksana also modeled energy and resource inputs and emissions from biomass life cycle stages and is incorporating profiles into a bio-energy with carbon capture and storage screening tool to evaluate key parameter sensitivities. Under the critical minerals effort, she compiled literature into a database summarizing state-of-the-science LCA and reviewed studies submitted to NETL from external projects. To support NETL's Gasification Systems Program, she characterized feedstocks for gasification and is currently developing a design basis for hydrogen production from biomass-fueled gasification.

Roksana earned a Ph.D. in Environmental Engineering and Earth Sciences from Clemson University, an M.S. in Chemical Engineering from Oklahoma State University and a B.S. in Chemical Engineering from Bangladesh University of Engineering and Technology. In her doctoral dissertation, she developed an integrated framework for simultaneous techno-economic and environmental evaluation of new products and processes, modeling the Clemson University Wastewater Treatment Plant as a case study.

// NOTICES

SSAE's Process Systems Engineering Research Team to Host SCGSR Fellowship Awardee

The Process Systems Engineering Research Team will host a Carnegie Mellon University (CMU) doctoral candidate over the summer under DOE's Office of Science Graduate Student Research (SCGSR) Program, which provides supplemental funds for graduate awardees to conduct part of their thesis research at a host DOE laboratory/facility in collaboration with a DOE laboratory scientist within a defined award period. CMU's William Strahl is one of 87 awardees from 58 different universities who will conduct research at 16 DOE national laboratories. His fellowship appointment will run from June 12 through September 18, 2023.

Strahl earned a bachelor's degree in chemical engineering from Brigham Young University with a minor in computer science before pursuing his doctorate at CMU under the guidance of Professor Chrysanthos Gounaris. His project will explore algorithms and parallel computing approaches for improving flowsheet initialization, frequently the most computationally expensive step in large-scale process optimizations. Strahl will work collaboratively with several IDAES researchers including Anthony Burgard, Andrew Lee* and John Eslick*.

LCA Team Conducts Carbon Conversion LCA Knowledge Sessions

Since 2019, SSAE's LCA Team has annually conducted CO_2 utilization (CO2U) LCA Knowledge Sessions to train DOE Carbon Conversion Program funding recipients in meeting requirements for completing LCAs of carbon conversion processes. Principal Investigators (PIs) explore these processes for their potential to reduce environmental emissions relative to alternatives by recycling waste CO_2 and transforming it into valuable products and applications.

Between February and April 2023, Michelle Krynock, Sheikh Moni* and Ben Young* provided six Knowledge Sessions in webinar format covering three distinct topics: 1) an overview of LCA basics and the NETL CO2U LCA Guidance Toolkit, 2) how to use modeling software openLCA to complete an LCA in conformance with the CO2U Guidance Document and 3) LCA results analysis and reporting. Each webinar involved a presentation including explanation, toolkit demonstrations and question-and-answer for PIs and other stakeholders.

The sessions navigated through the NETL CO2U LCA Guidance Toolkit. The toolkit provides a guidance document that outlines analysis requirements; a life cycle inventory database that includes unit process data and an example CO2U LCA; a results contribution tool for translating results from openLCA into final results; a data and modeling documentation spreadsheet; a report template and additional training resources such as a video series and subject matter expert support.

Want to learn more about SSAE's work?

Click here to see previous SSAE newsletter issues

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// PERSPECTIVES

SSAE Releases Updated Carbon Capture Retrofit Reports and Databases

Multiple products related to retrofitting PC and NGCC power plants with post-combustion carbon capture technology were recently released by SSAE. Included in the release were two technical reports that highlighted the cost and performance of the retrofitted plants and two carbon capture retrofit database (CCRD) spreadsheet tools. All products were updated to be consistent in methodology with the recently released Revision 4A to NETL's "[Cost and Performance Baseline for Fossil Energy Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity]" report (hereafter referred as "Baseline Study"). The tools provide stakeholders with conceptual-level cost and performance estimates for retrofitting the existing fossil fleet with solvent-based carbon capture technology.

One report, "[Cost and Performance of Retrofitting NGCC Units for Carbon Capture]," detailed the cost and performance of F- and H-frame NGCC plants retrofitted with post-combustion carbon capture. In this report, solvent-based (Shell CANSOLV) carbon capture technology was retrofitted onto an existing NGCC plant to capture 90, 95, or 97% of the CO_2 emissions. Being fully integrated, the plant supplies the necessary steam and power to meet the capture system's requirements.

Another report, "[Eliminating the Derate of Carbon Capture Retrofits]," detailed the cost and performance of subcritical PC plants retrofitted with Shell CANSOLV carbon capture technology to capture 90, 95, or 99% of the CO_2. In the report, several configurations were assessed including the fully integrated capture system (similar to the NGCC methodology) and two configurations that add separate natural gas-based systems to generate the necessary capture system power and/or steam.

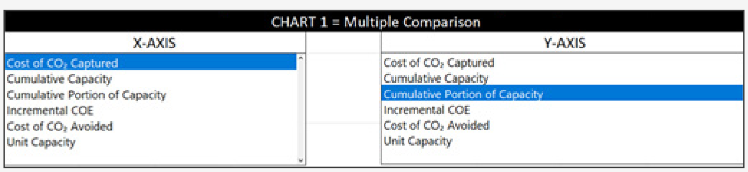
These options serve as a method to "eliminate" the plant derate by not extracting power and/or steam directly from the existing plant. In one configuration, a natural gas boiler was used to generate the necessary steam while the power was supplied by the existing plant. In the second configuration, a NGSC system generated combined heat (steam) and power (in excess) for the capture system.

Although techno-economic analyses of deep decarbonization (≥ 99%) of combustion flue gas have been published by others, the relatively limited experience with design and operation of capture systems that can routinely, reliably and economically achieve very high removal rates requires further study. In these reports, performance and cost estimations for the highest capture rates (97% for NGCC, 99% for PC) were reported in appendix material.

For each report, the retrofit cases were compared to analogous new build and non-capture cases assessed in the Baseline Study. A retrofit difficulty factor (RDF) was applied to scale costs, representing the difficulty associated with retrofitting an existing plant with new technology that it was not originally designed to incorporate. The primary metrics reported in each report compared the cost of capture (in $/tonne) and cost of electricity (in $/MWh) to Baseline Study cases. Several studies were conducted to determine the sensitivity of the cost of electricity to RDF, plant capacity factor, cost of natural gas, etc.

The results of these reports represent conceptual-level design and economic analysis, consistent with Association for the Advancement of Cost Engineering Class 4 estimation with -15/+25-30% uncertainty. The design basis for a specific real plant may deviate significantly from the cases assessed. Further analysis (e.g., a front-end engineering design study) is needed to produce budget-level cost estimates for carbon capture retrofits for a specific real facility. These reports did not consider maintenance or

Parameter	SCENARIO #1	
	Fleet Total	Unit Average
Total units, No.	693	–
Units retrofit with CCS, No.	505	–
Units retrofit with dry cooling, No.	106	–
Units retrofit with SCR, No.	343	–
Units retrofit with FGD, No.	246	–
Units retrofit with NGSC or NG Boiler, No.	0	–
Pre-retrofit capacity, MW	226,619	449
Pre-retrofit heat rate, Btu/kWh	–	10,755
Pre-retrofit CO_2 emissions, x1,000 TPY	1,053,535	2,059
Post-retrofit capacity, MW	160,997	319
Post-retrofit heat rate, Btu/kWh	–	14,987
Post-retrofit CO_2 emissions, x1,000 TPY	84,664	165
Retrofit CO_2 capture, x1,000 TPY	761,978	1,484
Retrofit parasitic load, MW	65,622	129.9
Makeup/excess power, x1,000 MW/yr	433,861	859.1
Retrofit capital cost (TOC), $/10⁶	593,147	1,175
Retrofit COE, $/MWh	–	288.5
Cost of CO_2 captured, $/tonne	–	225.4
Cost of CO_2 avoided, $/tonne	–	100.4
Scenario Assumptions:		
CO_2 capture rate, %	90%	
CO_2 capture technology	90% Cansolv	
Average pre-retrofit capacity factor	50%	
Average post-retrofit capacity factor	40%	
Retrofit unit capacity applicability limit, MW	25	
Retrofit cost factor	1.10	
Capital charge factor	0.077	
CO_2 emissions rate, lb/MMBtu	Varies	
Maximum CO_2 capture rate per train, TPD	15,772	
Plant capacity metric	Nameplate	
Cost year basis	2018	
Cooling preference	State	
Makeup/excess power costs/credits, $/MWh	N/A	
Include SCR with retrofit	Yes	
Include FGD with retrofit	Yes	
Additional heat rate penalty, Btu/kWh	N/A	
CO_2 transport and storage cost, $/tonne-$CO_2$	N/A	



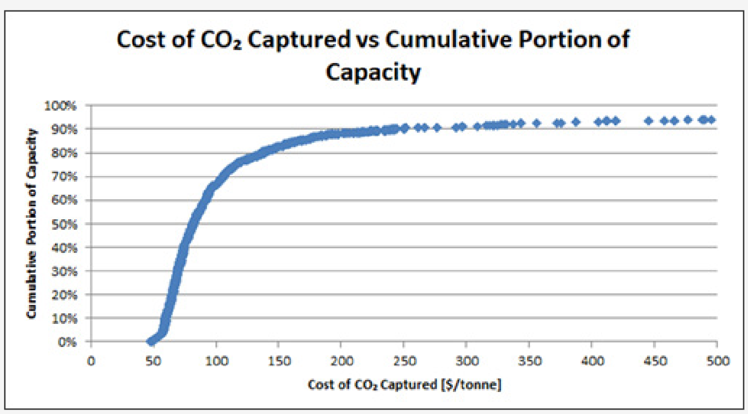


Figure 3. Sample output from the public version of the PC CCRD

// PERSPECTIVES (cont'd)

refurbishment that may be necessary to extend the life of the base plant such that it remains online for the 30-year economic lifetime assumed in estimating retrofit levelized cost of electricity and cost of capture.

The complementary CCRD tools are meant to supply end users with the means to estimate conceptual-level cost and performance details for user-defined power plants retrofitted with solvent-based carbon capture technology. These tools are based on the methodology employed in the reports discussed above and are subject to the same accuracy limitations. They are macro-based spreadsheet tools that calculate plant emissions, incremental cost of electricity and cost of carbon capture broken down into sub-categories (i.e., capital, variable, make-up power, etc.). The tools are customizable, allowing the end user to apply retrofit calculations to specific plant(s) of interest (user defined plant characteristics).

The tools are available for PC (Pulverized Coal CCRD) and NGCC (Natural Gas Combined Cycle CCRD) plants (with a similar tool also available for industrial capture [Industrial Sources CCRD] published last year). Embedded in the spreadsheet tools is a user guide, "User Guide for the Public Power Generation CO_2 Capture Retrofit Database Models," that explains in detail the functionality of the tools to end users. The user guide for the Industrial Sources CCRD is embedded within the CCRD but also published as a separate file on NETL's website. A sample of the PC CCRD output is given in Figure 3. Several SSAE researchers contributed to the PC, NGCC and industrial retrofit products including Gregory Hackett, Kyle Buchheit*, Sally Homsy*, Tommy Schmitt*, Norma Kuehn*, Mark Woods*, Tim Fout, Travis Shultz, Sydney Hughes*, Alex Zoelle*, Samuel Henry*, Sandeep Pidaparti* and Eric Grol. – Contributed by Gregory Hackett

// UPCOMING CONFERENCES AND EVENTS

SSAE federal staff and NETL support contractor personnel attended or presented in May 2023 and will attend or present in June and July 2023 at the following conferences:

- Offshore Technology Conference 2023
  Participants: Luciane Cunha and Timothy Grant
  Houston, TX, May 1–4, 2023
- Joint NRAP-SMART-EDX4CCS Technical Meeting
  Presenter: David Morgan – 1) Quantifying Liability and Life Cycle Cost of Risk–Building a New Computational Module to Link Risk, Risk Management, and Cost and 2) Integration of Economic and Risk Modules with ML-Based Tools (co-presenter)
  Participant: Travis Warner*
  Santa Fe, NM, May 2–4, 2023
- AISTech 2023
  Participant: Eric Grol
  Detroit, MI, May 8–11, 2023
- NAWI External Peer Review
  Presenter: Timothy Bartholomew – Water treatment Technoeconomic Assessment Platform (WaterTAP)
  Berkeley, CA, May 9, 2023
- NERC Energy Assurance with Energy-Constrained Resources, Standards Drafting Team Meeting
  Participant: John Brewer
  Hybrid (Virtual and Atlanta, GA), May 9–10, 2023
- Critical Minerals & Materials (CMM) Mini-Symposium
  Presenter: Thomas Tarka – PrOMMiS: Applying Novel Modeling Methods to Accelerate Critical Minerals RD^3 (poster)
  Arlington, VA, May 15, 2023
- World Hydrogen North America 2023
  Participant: Peter Balash
  Houston, TX, May 15–17, 2023
- Spring National Carbon Capture Center Meeting
  Participant: Timothy Fout
  Birmingham, AL, May 16–17, 2023
- 2023 CCUS TEA/LCA Workshop on Harmonizing CCUS Assessments
  Presenter: Michelle Krynock – Carbon Conversion Life Cycle Analysis at NETL
  Co-moderator: Michelle Krynock – Utility of Geospatial Analysis session
  Participants: Roksana Mahmud* and Shirley Sam*
  Hybrid (Virtual and Ann Arbor, MI), May 16–18, 2023
- Carbon Intel Forum 2023
  Participants: Peter Balash and Luciane Cunha
  Houston, TX, May 23–24, 2023
- 18th International Symposium on Solid Oxide Fuel Cells (SOFC-XVIII)
  Presenter: Gregory Hackett – SOFC-0376–Techno-Economic Analysis of Reversible and Paired Solid Oxide Cell Systems for Hydrogen Production
  Co-chair: Gregory Hackett – 1) SOFC–Characterization and Testing 2, 2) SOFC–Characterization and Testing 3 and 3) SOFC–Durability/Reliability and Degradation Mechanisms 1 sessions
  Boston, MA, May 28–June 2, 2023

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UPCOMING CONFERENCES AND EVENTS (cont'd)

- Annual Merit Review and Peer Evaluation Meeting – U.S. Department of Energy Hydrogen Program
  Presenters: Anthony Burgard – FE017 Technoeconomic Evaluation of SOFC/SOEC-Based Integrated Energy Systems for the Co-Production of Electricity and Hydrogen (poster) and Alexander Dowling* – FE020 Market-Based Technoeconomic Optimization of Integrated Energy Systems that Co-Produce Hydrogen and Electricity
  Participants: Shannon McNaul* and Robert Stevens
  Hybrid (Virtual and Arlington, VA), June 5–8, 2023
- I-West Seminar
  Co-presenter: Derek Vikara – Pathways to CO_2 Utilization and Storage for the Intermountain West
  Virtual, June 7, 2023
- International Symposium on Sustainable Systems and Technology (ISSST) 2023 Conference
  Presenter: Harshvardhan Khutal* – Evaluating U.S. Natural Gas Environmental Performance
  Participants: Derrick Carlson* and Shirley Sam*
  Fort Collins, CO, June 12 (pre-conference workshops) and 13–15 (conference), 2023
- Snowmass Week 1 "The Pace of Climate Action in a World of Multiple Priorities" Workshop
  Participant: Timothy Fout
  Snowmass Village, CO, June 19–23, 2023
- Mineral-X Launch Symposium – "Critical Minerals: efficient exploration and responsible mining"
  Participant: Alison Fritz
  Stanford, CA, June 20–21, 2023
- 15th Lithium Supply and Battery Raw Materials 2023
  Participant: Alison Fritz
  Las Vegas, NV, June 20–22, 2023
- NERC Energy Assurance with Energy-Constrained Resources, Standards Drafting Team Meeting
  Participant: John Brewer
  Virtual, June 22 and 29, 2023
- ASME Turbo Expo 2023
  Presenter: Eric Liese – Modeling a Water-Cooled Printed Circuit Heat Exchanger Condensing CO_2 for Use in sCO_2 Cycle System Optimization Studies
  Boston, MA, June 26–30, 2023
- Hydrogen Technology Expo North America 2023
  Participant: Eric Lewis
  Houston, TX, June 28–29, 2023
- NERC Energy Assurance with Energy-Constrained Resources, Standards Drafting Team Meeting
  Participant: John Brewer
  Virtual, July 6, 2023
- Berkeley Workshop: Past, Present, and Future of Diversity in Computing
  Participant: Markus Drouven
  Berkeley, CA, July 7, 2023
- 17th International Conference on Energy Sustainability
  Presenter: Thomas Tarka – Process-Based Cost Estimation Framework for Assessing Economic Viability of Environmentally and Socially Sustainable Rare Earth Element Feedstocks
  Washington, D.C., July 10–12, 2023
- 2023 AAEA Annual Meeting
  Participant: Amanda Harker Steele
  Washington, D.C., July 23–25, 2023
- 47th International Technical Conference on Clean Energy – The Clearwater Clean Energy Conference
  Presenter: Robert Stevens – Bioenergy Carbon Capture and Storage (BECCS): Integrated Power Plant System Study
  Co-chair: Robert Stevens
  Participant: Benjamin Omell
  Clearwater, FL, July 23–27, 202

RECENT PUBLICATIONS

Articles

- R. Jacobs, J. Liu, B. Tak Na, B. Guan, T. Yang, S. Lee, G. Hackett, T. Kalapos, H. Abernathy and D. Morgan, "Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies," *Advanced Energy Materials*, vol. 12, no. 25, article 2201203, July 7, 2022.
- Y. Lee, Y. Duan, D. Sorescu, W. Saidi, D. Morgan, K. Thomas, W. Epting, G. Hackett and H. Abernathy, "Defect Thermodynamics and Transport Properties of Proton Conducting Oxide $BaZr_{1-x}Y_xO_{3-\delta}$ ($x \leq 0.1$) Guided by Density Functional Theory Modeling," *JOM*, vol. 74, no. 12, pp. 4506-4526, December 2022.
- J. Wang and A. Dowling, "Pyomo.DOE: An open-source package for model-based design of experiments in Python," *AIChE Journal*, vol. 68, no. 12, e17813, December 2022.

RECENT PUBLICATIONS cont'd

- P. Akula, A. Lee, J. Eslick,, D. Bhattacharyya and D. Miller, "A modified electrolyte non-random two-liquid model with analytical expression for excess enthalpy: Application to the MEA-H_2O-CO_2 system," *AIChE Journal*, vol. 69, no. 1, e17935, January 2023.
- K. Bello, D. Vikara, A. Sheriff, H. Viswanathan, T. Carr, M. Sweeney, D. O'Malley, M. Marquis, R. Taylor Vactor and L. Cunha, "Evaluation of the economic implications of varied pressure drawdown strategies generated using a real-time, rapid predictive, multi-fidelity model for unconventional oil and gas wells," *Gas Science and Engineering*, vol. 113, article 204972, May 2023.
- A. Harker Steele, S. Sharma, I. Pena Cabra, L. Clahane and A. Iyengar, "A tool for measuring the system cost of replacement energy," *Energy*, vol. 275, article 127394, July 15, 2023.
- M. Drouven, D. Cafaro and I. Grossmann, "Mathematical Programming Models for Shale Oil & Gas Development: A Review and Perspective," *Computers & Chemical Engineering*, vol. 177, article 108317, September 2023.

Database

- National Energy Technology Laboratory, "Pulverized Coal CO_2 Capture Retrofit Database (PC CCRD)," National Energy Technology Laboratory, Pittsburgh, PA, March 2023.

Reports/Supporting Documentation

- T. Shultz, E. Lewis, A. O'Connell, S. Hughes and M. Woods, "Development of Advanced Ultra-Supercritical (AUSC) Pulverized Coal (PC) Plants," National Energy Technology Laboratory, DOE/NETL-2020/2152, Pittsburgh, PA, November 11, 2020.
- K. Bello, D. Vikara, A. Sheriff, H. Viswanathan, T. Carr, M. Sweeney, D. O'Malley, M. Marquis, R. Taylor Vactor and L. Cunha, "Supplementary Data for Evaluation of the Economic Implications of Varied Pressure Drawdown Strategies Generated Using a Real-time, Rapid Predictive, Multi-fidelity Model for Unconventional Oil and Gas Wells by Bello, K., Vikara, D., Sheriff, A., Viswanathan, H., Carr, T., Sweeney, M., O'Malley, D., Marquis, M., Vactor, R.T., and Cunha, L.," DOI: 10.18141/1894134, 2022.
- A. Fritz, C. Able, M. Mauter and E. Grol, "Supporting Information for Aqueous Bromide Discharges from U.S. Coal-Fired Power Plants: Points of Origin, Concentration Ranges, and Effluent Treatment Costs," supporting information (final presentation), 2023.
- M. Turner, T. Schmitt, M. Oakes, J. Konrade, M. Bleckinger and M. Sturdivan, "Cost and Performance Baseline for Fossil Energy Plants, Volume 3: Low Rank Coal and Natural Gas to Electricity", National Energy Technology Laboratory, DOE/NETL-2023/3852, Pittsburgh, PA, March 20, 2023.
- K. Buchheit and N. Kuehn, "Eliminating the Derate of Carbon Capture Retrofits – Revision 2," National Energy Technology Laboratory, DOE/NETL-2023/3850, Pittsburgh, PA, March 31, 2023.
- S. Hughes and P. Cvetic, "Analysis of Carbon Capture Retrofits for Cement Plants," National Energy Technology Laboratory, DOE/NETL-2023/3856, Pittsburgh, PA, March 31, 2023.
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- M. Krynock, "Carbon Conversion Life Cycle Analysis at NETL," presentation at the 2023 CCUS TEA/LCA Workshop on Harmonizing CCUS Assessments, Hybrid (Virtual and Ann Arbor, MI), May 18, 2023.

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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
- Life Cycle Analysis

- SSAE website
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