SSAE Newsletter

DECEMBER // 2022 VOLUME 2.11

// 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

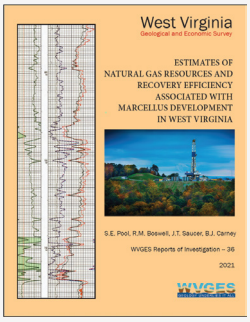
Study Shows Variations in Natural Gas Delivery Pathway Emissions

A paper showing variations in life cycle greenhouse gas (GHG) emissions from the natural gas supply chain depending on where natural gas is produced and consumed was co-authored by SSAE Life Cycle Analysis (LCA) Team researcher Timothy Skone and published in *Environmental Science & Technology*. Results from production and consumption scenarios in this study can help inform options for reducing GHG emissions from the natural gas supply chain.

An algorithm that pairs specific production basins to delivery regions by optimizing the shortest average natural gas transportation distance was developed. The study subdivided data and results into six transmission and distribution regions: Pacific, Rocky Mountain, Southwest, Midwest, Southeast and Northeast. NETL's life cycle natural gas model enhanced with natural gas production and delivery volumes for each state, weighted geographical centers for processing and delivery locations and regional emissions factors for commercial and industrial meters was used to calculate GHG emissions from production through delivery.

Delivery to the Pacific region yielded the highest expected life cycle GHG emissions in units of grams of carbon dioxide (CO_2) equivalents per megajoule of natural gas delivered (13.0 g CO_2e/MJ), while delivery to the Northeast United States yielded the lowest expected life cycle GHG emissions (8.1 g CO_2e/MJ).

SSAE Contributes to Award-Winning Report

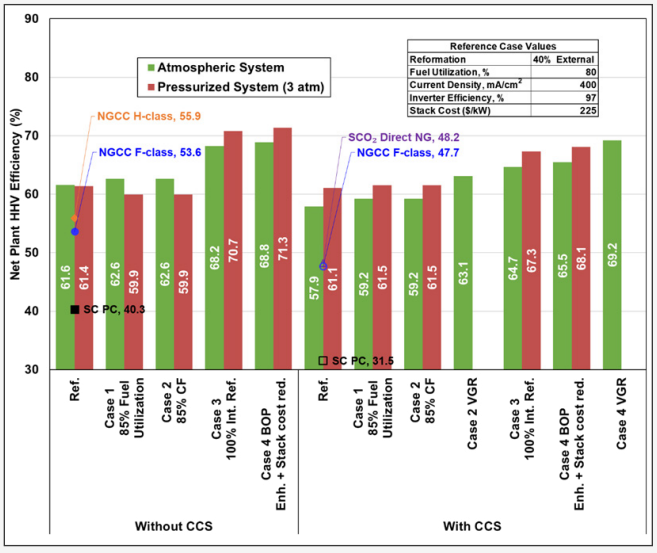


The report, "Estimates of Natural Gas Resources and Recovery Efficiency Associated with Marcellus Development in West Virginia," (i.e., West Virginia Geological & Economic Survey [WVGES] Reports of Investigation RI-36) was recently awarded the 2022 "Charles J. Mankin Memorial Award" by the Association of American State Geologists. The award is given each year to a report led by a state geologic survey that "elegantly, thoroughly and innovatively provides sound and influential information on regional geology or an energy or mineral resource topic." Part of a collaboration between NETL/SSAE, WVGES and Northeast Natural Energy, this report was designed to develop new procedures to assess gas resources and recovery efficiency in Appalachian basin shale reservoirs. Five publications were released, beginning with WVGES Reports of Investigation RI-35 which outlined the geology of the units that contribute to production from Marcellus development. SPE-201752 described a new method for resource assessment focused on normalization of well productivity from representative multi-well developments as normalized for both well lateral length and well spacing. WVGES Reports of Investigation RI-36 (winner of the Mankin Memorial Award) applied this method to the Marcellus of West Virginia and reported that prevailing estimates of both resource availability and recovery efficiency are significantly low. A 2021 NETL report, "Evaluation of Technically-Recoverable Resources in the Marcellus and Utica Shale Gas Plays of the Appalachian Basin," extended the methodology throughout the Appalachian basin for both the Marcellus and Utica shale plays. In late 2021, the team was invited to provide a summary report of the effort in the *Oil & Gas Journal*.

Revised NGFC Pathway Study Released

NETL has published an updated analysis of the potential performance and costs for advanced natural gas-fueled solid oxide fuel cell (SOFC) power generation systems. The report, "Techno-Economic Analysis of Natural Gas Fuel Cell Plant Configurations," details multiple SOFC plant configurations, primarily distinguished by the inclusion of carbon capture and fuel cell stack pressurization. The study focuses on utility-scale power plant systems that are aligned with long-term market opportunities to provide secure and reliable dispatchable generation at high efficiency and carbon capture rates. While significant technical challenges for the wide-scale deployment of SOFC technology remain (e.g., reliability, performance stability/degradation, cost at low production volumes), the technology does have the potential, with successful development, to be the most efficient and environmentally friendly fossil fuel-based power generation technology.

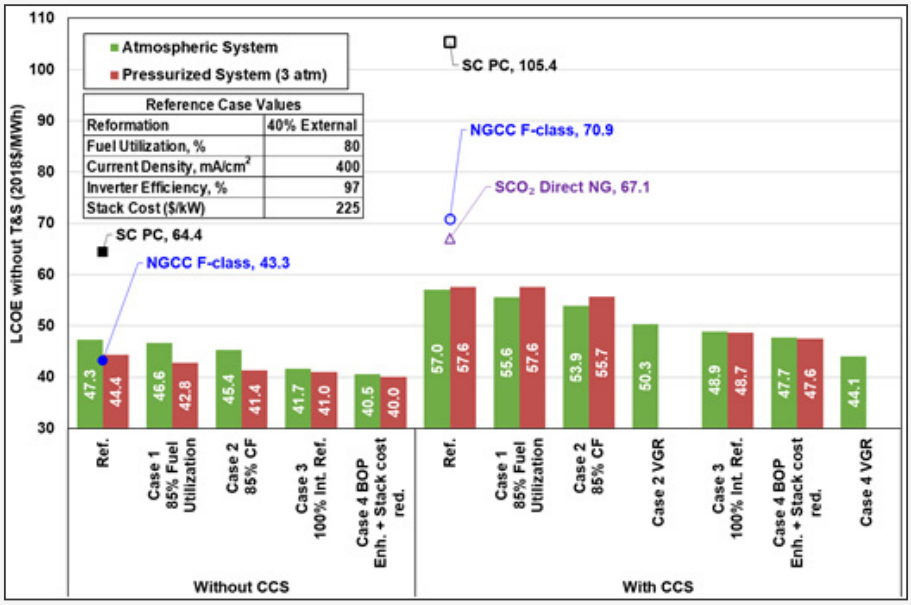
The natural gas fuel cell (NGFC) pathway examines the potential cost and performance of SOFC systems as the technology matures. Targeted improvements to major subsystems are identified and the impact assessed. Compared to commercial natural gas combined cycle (NGCC) plants, SOFC technology has the potential to lower both electricity and carbon capture costs. NGFC systems show anywhere between a 7 and 20 percentage point improvement in higher heating value (HHV) efficiency, depending on the case, with most NGFC systems in the 60-70% efficiency range (see figure below).



HHV efficiency of the pathway NGFC plants, atmospheric and pressurized both with and without carbon capture

// HIGHLIGHTS cont'd

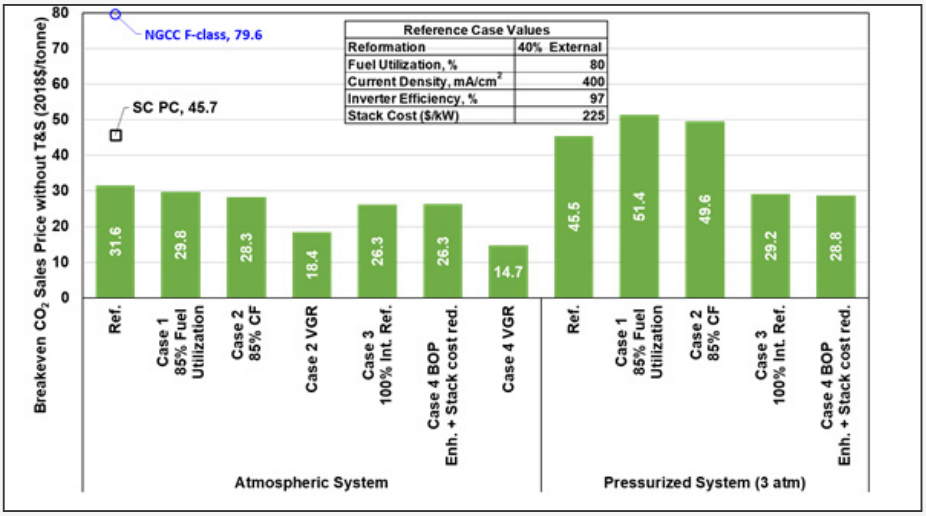
While unabated NGFC systems may be competitive with NGCCs with respect to levelized cost of electricity (LCOE), it is with carbon capture that the potential benefit is most evident (see figure below). Taking advantage of SOFCs' very high efficiency (because it is not a heat engine, it is not subject to Carnot limitations) and process intensification (in addition to power generation, the SOFC serves as an oxygen transport membrane and steam-methane reformer in certain cases), LCOE ranges from ≈$23–60/MWh lower than 90% carbon capture and storage (CCS) NGCC systems. Since the oxidant and fuel are separated in a fuel cell, any unutilized fuel exiting the stack can be oxy-combusted which allows for the use of a CO_2 purification unit (CPU) instead of a solvent-based capture system. All of the NGFC cases with carbon capture examined in this study exceed 90% CCS.



Comparison of the LCOE (without transport and storage [T&S]) of the NGFC plants

Advanced fuel cell technology combining high efficiency and low-cost systems lead to a major potential role in decarbonizing the energy sector. NGFC systems have the potential for break-even CO_2 sales prices that are well below $40/tonne. A system featuring vent gas recirculation (VGR) even has the potential to bring this cost of capture down to lower than $15/tonne (see figure below). Ninety percent CO_2 capture was chosen as a basis of comparison for the NGCC systems where the NGFC configurations can capture upwards of 98% due to the combination of oxy-combustion and the CPU.

This work has served as the basis for many other NETL SOFC based studies and lays the groundwork for future techno-economic analysis (TEA) of different fuel cell technology-based systems including reversible solid oxide cells, hydrogen-fueled fuel cells and various hybrid systems that include electrolysis.



Break -even sales price of CO_2 captured for the different NGFC plant configurations

// HIGHLIGHTS cont'd

SSAE'S Energy Market Analysis Team Develops ES Database

An interactive, web-based database of energy storage (ES) assets co-located with existing fossil energy (FE) power technologies ("ES-FE Database") was developed by SSAE's Erik Shuster, Ivonne Pena-Cabra*, Smriti Sharma*, Clare Callahan* and Kirtan Jani*. The database combined data from several public resources including the Energy Information Administration-860 dataset, Sandia National Laboratories' ("Sandia") Global Energy Storage Database, Lawrence Berkeley National Laboratory's (LBNL) Online Hybrid and Energy Storage Projects Dataset and three additional projects from a web search of potential FE repurposed assets. The concepts listed in the ES-FE Database correspond to the 29 awarded projects under DOE Funding Opportunity Announcement (FOA) 2332 Phase I and the three awarded projects under Phase II.

The ES-FE Database is publicly available and is part of a journal paper (submitted to *Applied Energy* for consideration) titled "Market analysis for the integration of new power technologies: a case study of the deployment of hybrid fossil-based generator plus energy storage (ES-FE)," which describes and quantifies region-specific market conditions for the deployment of ES-FE. This is the first database that exclusively applies to FE power plants that have already added ES to their assets and to the sector, which is exploring innovative concepts. The tool has two main tabs, a map tab and a table tab. The map geolocates over 65 concepts and projects and gives the user the option to group the projects by data source, project type and power/ES technology. The table tab provides the user with the flexibility to copy attribute data.

Staff Spotlight

Since joining the Process and Cost Engineering team in January 2021, Sam Henry* has primarily supported work under Carbon Conversion. He has completed screening techno-economic analyses (TEA) on novel carbon conversion technologies under development by NETL's Research and Innovation Center, including a microwave-assisted catalyst for the conversion of CO_2 and methane to syngas and a biological catalyst for the conversion of CO_2 to acetic acid. Sam has also advanced the development of guidance tools that support TEA of carbon conversion technologies including the forthcoming guidance document, "Quality Guidelines for Energy System Studies: Performing a Techno-Economic Analysis for CO_2 Conversion Technologies," and a public web-based toolkit that will include this guidance document as well as supplementary tools to assist technology developers, NETL researchers and relevant stakeholders in completing carbon conversion TEA.

Sam is from the Pittsburgh area and graduated from Carnegie Mellon University (CMU) in 2020 with a B.S. in Chemical Engineering and a minor in Social and Political History. He previously completed an internship with Total Equipment Company in 2019 as a sales engineer.

// NOTICES

IDAES Stakeholder Workshop Showcases Advances and Applications

The annual Institute for the Design of Advanced Energy Systems (IDAES) Stakeholder Workshop was held in-person in Washington, DC in September 2022. Twenty-five stakeholders from industry, DOE/FECM and academia attended the event. The keynote address was delivered by NETL Director Brian Anderson (learn more). Oral presentations were delivered by several members of the IDAES Technical Team, including:

- *IDAES Program Overview*. David Miller (NETL) described how IDAES is well positioned to be a core contributor to high-level national energy system objectives such as economy-wide decarbonization and the accompanying energy transition.
- *Growth and Development of the IDAES Integrated Platform*. Andrew Lee* discussed 1) the need to balance demands for new features with interface stability, testing and verification and 2) how IDAES is now a stable platform which supports cutting edge optimization tools with a growing library of process models and an active user community.
- *User Interfaces and User Support*. Dan Gunter (LBNL) described significant improvements to the IDAES Flowsheet Visualizer as well as new debugging tools, re-organized documentation for easier navigation and several channels for user support.

* NETL Support Contractor

// NOTICES cont'd

- *Surrogate Modeling for Improved Design and Operations*. Carl Laird (CMU) covered the continued development of an extensive collection of surrogate modeling tools, including streamlined workflows and a unified application programming interface (API) to facilitate their use.
- *Optimization of Grid-Integrated Processes for Decarbonization*. Alex Dowling (Notre Dame University) described how IDAES has developed a unique capability to simulate both the grid and its components as well as their interactions.
- *Integrated Energy Systems for Power and Hydrogen*. Tony Burgard (NETL) presented an integrated process/market analysis demonstrating that flexible power and hydrogen systems based on SOFC and solid oxide electrolysis cell technologies are especially attractive in scenarios with bimodal electricity prices.
- *Design and Operation of Flexible Carbon Capture for Dynamic Energy Systems*. Jaffer Ghouse* described a new capability to evaluate flexible carbon capture technologies in the context of regional electricity markets which was developed through the Advanced Research Projects Agency-Energy's (ARPA-E) FLExible Carbon Capture and Storage (FLECCS) program in collaboration with Svante, Susteon, the Southern California Gas Company (SoCalGas) and the Los Angeles Department of Water and Power.
- *Mitigating Technical Risk with Robust Design and Uncertainty Quantification*. Chrysanthos Gounaris (CMU) described an End-to-End Framework for Risk-Averse Process Design, which integrates various tools to enable decision makers to avoid unnecessary overdesigns and shorten development cycles. He also described the new Pyomo Robust Optimization Solver (PyROS) for two-stage nonlinear robust optimization.
- *Optimal Long-Term Expansion Planning of Power Generation Systems*. Ignacio Grossmann (CMU) presented new research that optimizes reserve capacity in an expansion planning model and considers a dual role for backup generators – remaining as a backup to increase reliability and generating electricity to meet power demand.
- *Application to Water Management, Treatment, and Desalination: WaterTAP and PARETO*. Tim Bartholomew and Markus Drouven (both NETL) described how IDAES tools are supporting evaluation of water purification and produced water processing technology options.

Industry stakeholder presentations and a panel discussion also provided opportunities for the stakeholders to share their recent experiences in applying the IDAES platform as well as advice on how to maximize its impact going forward. Workshop materials will be accessible to IDAES stakeholders through the IDAES website and can be made available upon request.

LCA Researchers Present at LCA Conference

SSAE LCA Team researchers presented work at the American Center for Life Cycle Assessment (ACLCA) 2022 Conference in November 2022:

- An overview of projects advanced by NETL and categorized under LCA expert and review support, decarbonization and sustainability, emerging technology and evaluation, advancing LCA capabilities and establishing national baselines was presented by Timothy Skone.
- A new tool designed to send data from ElectricityLCI, which is NETL's life-cycle dataset for U.S. electricity consumption and generation, to air quality, water scarcity and chemical and environmental impact assessment methods was presented by Tyler Davis*. The tool allows users to customize the inventory data to assess current and future electricity generation mixes.
- In the research area of CO_2 utilization, an LCA of microwave-assisted catalytic conversion of CO_2 to methanol, which can be directly utilized or converted into other chemicals, was presented by Joseph Chou*. This study provides a starting point for future investigation into other pathways for converting CO_2 into valuable products.
- Research on building materials manufactured by reacting waste materials (steel slag) with CO_2 was described by Sheikh Moni*. In addition, Moni co-led a special session titled "Life Cycle Assessment of Emerging Technologies: Update on the SETAC/ACLCA Working Group Progress." The Society of Environmental Toxicology and Chemistry (SETAC)/ACLCA Working Group seeks to improve the LCA of emerging technologies by addressing technical and methodological issues.

// UPCOMING CONFERENCES AND EVENTS

SSAE Federal staff will attend the following event in December 2022:

New Mexico Produced Water Research Consortium Workshop (Non-public)
Participant: Markus Drouven
Albuquerque, NM, December 6, 2022

// RECENT PUBLICATIONS

Manuscripts

- M. G. Drouven, A. J. Calderon, M. A. Zamarripa and K. Beattie, "PARETO; An open-source produced water optimization framework", *Optimization and Engineering*, November 4, 2022.
- K. Hedrick, E. Hedrick, B. Omell, S. E. Zitney and D. Bhattacharyya, "Dynamic Modeling, Parameter Estimation, and Data Reconciliation of a Supercritical Pulverized Coal-Fired Boiler," *Industrial & Chemical Engineering Research*, vol. 61, no. 45, pp. 16764–16779, November 7, 2022.

Reports/Supporting Documentation

- M. Mauter, A. Mulchandani and A. Fritz, " Impact of Non-Steady State Operation on Cooling Water Consumption at Coal- And Natural Gas-Fired Power Plants," National Energy Technology Laboratory, DOE/NETL-2021/2884, Pittsburgh, PA, January 14, 2021.
- D. Morgan, A. Guinan, T. Warner, D. Vikara and R. T. Vactor, "Intermountain West Energy Sustainability & Transitions Initiative: CO_2 Transport and Geologic Storage Modeling Results," DOI: 10.18141/1890177, 2022.
- A. Wendt, A. Sheriff, C. Shih, D. Vikara and T. Grant, "A Multi-criteria CCUS Screening Evaluation of the Gulf of Mexico, USA – Supplementary Data," DOI: 10.18141/1806193, 2022.
- T. Warner, D. Vikara, E. Basista and T. Grant, "Evaluating the Impacts of the Bipartisan Budget Act of 2018 45Q Tax Credit on CCS Network Costs," National Energy Technology Laboratory, DOE/NETL-2022/3816, Pittsburgh, PA, September 27, 2022.
- E. Shuster, K. Kern and P. Balash, "NETL Energy Related Diagrams – 2021 Edition," National Energy Technology Laboratory, DOE/NETL-2022/3260, Pittsburgh, PA, December 6, 2022.

Conference Proceedings and Events

- S. Moni, "Life Cycle Analysis of Emerging Technologies," guest lecture for advanced LCA class at The Pennsylvania State University, State College, PA, October 18, 2022.
- M. Drouven and M. Zamarripa-Perez, "Project PARETO – DOE's Produced Water Optimization Initiative," presentation at the 2022 Resource Sustainability Annual Project Review Meeting, Pittsburgh, PA, October 25, 2022.
- A. J. Harker Steele, "Barriers and Opportunities for Carbon Capture, Utilization, & Storage (CCUS) in Achieving a Net Zero Emissions Future – System Cost of Replacement Energy (SCoRE): A Tool for Assessing Technology Substitution Pathways to Decarbonization," presentation at the 39th Annual USAEE/ IAEE Conference during the "Barriers and Opportunities for CCUS" session, Houston, TX, October 25, 2022.
- J. Liu , R. Jacobs , B. Guan, T. Yang, R. Pineault, T. Kalapos, G. Hackett, H. Abernathy and D. Morgan, "Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- W. K. Epting, Y. Lei, J. H. Mason, T. Kalapos, G. A. Hackett and H. Abernathy, "Rapid Assessment of SOC Electrode Degradation Using Computer Vision and Machine Learning," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- Y. Fan, Y. Chen, R Pineault, R. Addis, B. Guan, H. Abernathy, X. Song, G. Hackett and T. Kalapos, "Nanoparticles Infiltration in Air Electrode of LSM-YSZ/YSZ/Ni-YSZ Cells to Improve Performance and Mitigate Performance Degradation under Reversible SOFC/SOEC Operation," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- H. Kim, A. D. Rollett, P. A. Salvador, W. K. Epting, H. Abernathy and G. Hackett, "Effects of Microstructural Variability and Operating Conditions on Cr-poisoning in Solid Oxide Fuel Cell Cathodes Using High-Performance Computing Simulations," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- Y. Lei, Y. Lee, W. K. Epting, J. H. Mason, T. Cheng, H. Abernathy, G. Hackett, and Y. Wen, "Modeling Ni redistribution in the fuel electrode of solid oxide cells," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- Y. Lee, Y. Duan, D. Sorescu, W. Saidi, D. Morgan, W. K. Epting, T. Kalapos, G. A. Hackett and H. Abernathy, "Defect Thermodynamics and Transport Properties of Proton Conducting Oxide $BaZr_{1-x}Y_xO_{3-\delta}$ ($x \leq 0.1$) Evaluated Based on Density Functional Theory Modeling" poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- Y. Chen, Y. Fan, H. Abernathy, G. Hackett and X. Song, "Surface & Grain Boundary Degradation of LSCF/SDC Electrode in SOFC and SOEC," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.

// RECENT PUBLICATIONS cont'd

- T. Yang, B. Guan, J. Liu, Y. Fan, H. Finklea, W. K. Epting, H. W. Abernathy, G. A. Hackett and T. L. Kalapos, "Numerical Study to Optimize the Microstructure of an LSM/YSZ Backbone for Nanoparticle Infiltration," poster at the 23rd Annual Solid Oxide Fuel Cell Program Project Review Meeting, Coraopolis, PA, October 25–27, 2022.
- M. Stuckman, "Characterization-Informed Recovery of Critical Minerals from Acid Mine Drainage Treatment Solids – FWP-1022420," presentation at the 2022 Resource Sustainability Annual Project Review Meeting, Pittsburgh, PA, October 27, 2022.
- M. Jamieson, "LCA Tools Available at NETL," presentation at the kick-off meeting for FOAs 2596 and 2598 – University Training and Research for Fossil Energy and Carbon Management – UCR and Minority Serving Institutions, Virtual, November 1, 2022.
- T. Bartholomew, "Water Treatment Technoeconomic Assessment Platform (WaterTap)," NAWI Tools Deep Dive, presentation at the NAWI Alliance Fall Meeting 2022 (Day 1), Virtual, November 1, 2022.
- T. Bartholomew, "Water Treatment Technoeconomic Assessment Platform (WaterTap)," presentation at the NAWI Alliance Fall Meeting 2022 (Day 2), Virtual, November 2, 2022.
- T. J. Skone and M. Jamieson, "U.S. DOE Special Session: National Energy Technology Laboratory LCA Update," presentation at the ACLCA 2022 Conference, Virtual, November 8, 2022.
- S. Moni, S. Chauhan, J. Chou, M. Krynock and T. J. Skone, "Life Cycle Analysis of CO_2-Derived Building Materials: CO_2-cured Concrete and Building Aggregates," presentation at the ACLCA 2022 Conference, Virtual, November 10, 2022.
- S. Moni, M. Krynock and T. Skone, "Life Cycle Analysis Tools to Determine Environmental Footprint of Carbon Utilization Projects," presentation at the 2022 AIChE Annual Meeting during the "Novel Approaches to CO_2 Utilization I" session, Phoenix, AZ, November 14, 2022.
- M. Turner, M. Oakes, J. Konrade, M. Bleckinger, S. Hughes and T. Shultz, "Conceptual Design of Pulverized Coal Electricity Generating Units for Flexible Operation," presentation at the International Centre for Sustainable Carbon's workshop "The Energy Transition – The Role for Sustainable Carbon," Hybrid (Virtual and Sardinia, Italy), November 17, 2022.
- E. Lewis, "TEA and LCA Assessments of H_2 Production from Coal, Coal/Biomass, and Biomass," presentation at the Gasification Technology Status and Pathways for Net-Zero Carbon Economy Workshop, Virtual, November 30, 2022.

// 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

Life Cycle Analysis Models

NETL LCA CO2U 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

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