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

NETL AI Image Embedding Tool Promising for Greater Understanding of the Subsurface

SSAE and other NETL researchers, in a case study, have demonstrated the power of their artificial intelligence (AI)-informed image embedding tool. Using visual information from over 1,000 documents—including unstructured data (such as maps, publications, reports, presentations) related to the Gulf of Mexico—as input, the tool accurately labels and organizes images with 90–95% precision in less than ten minutes (Figure 1). The case study was recently published in the journal Frontiers in Big Data under the title "Enhancing knowledge discovery from unstructured data using a deep learning approach to support subsurface modeling predictions." The tool is part of a software suite that emerged from the Lab's Subsurface Trend Analysis (STA) workflow and was developed by NETL researchers Brendan Hoover*, Dakota Zaengle*, Patrick Wingo, Anuj Suhag*, Kelly Rose, and SSAE's MacKenzie Mark-Moser. Learn more

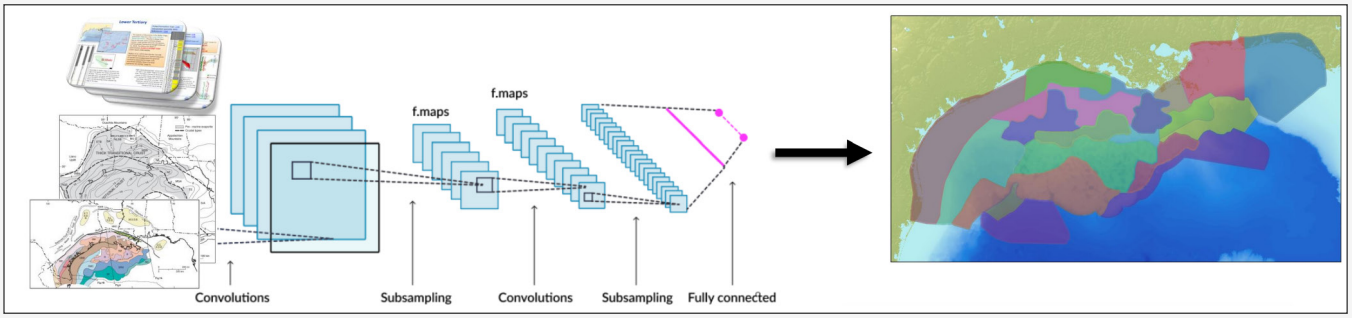

Figure 1. Schematic of Convolutional Neural Network training for image identification

NETL's Electrochemical Conversion of CO_2 Sensitivity Analysis Tool

SSAE researchers have developed the NETL Electrochemical Conversion of CO_2 Sensitivity Analysis Tool and accompanying user guide, enabling analysis of the impacts of changing design assumptions for an electrochemical conversion (ECC) system that converts CO_2 to value-added products via electrochemical reduction using catalyst materials on the cathode to promote the conversion.

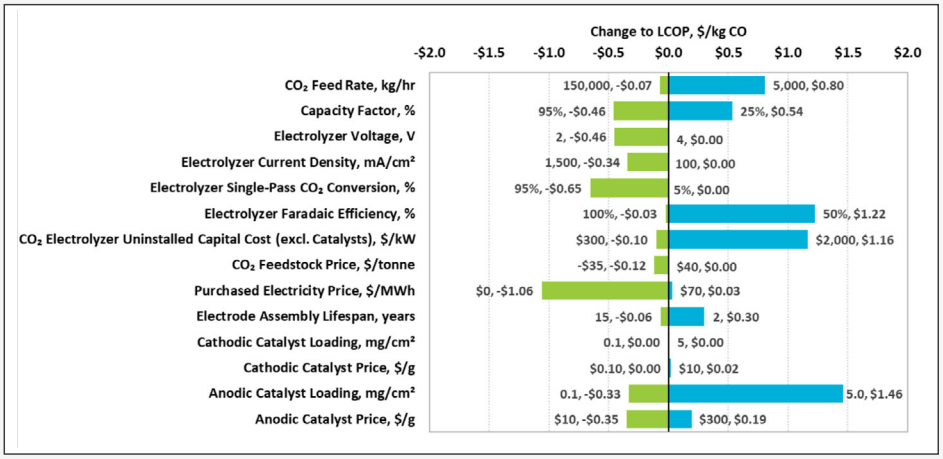

Figure 2. Example of the impact of design assumption changes on the levelized cost of production (LCOP) of CO

Manipulable input values and sensitivity ranges allow users to tailor the tool outputs to project-specific needs. Results are presented in several tabular and graphical formats, such as the tornado plot, Figure 2, which depicts changes to the levelized cost of production (LCOP) of CO at the specified low- and high-cost sensitivity bounds of select design assumptions. Researchers may use such sensitivity analyses and the resulting cost and performance calculations to guide R&D toward advancements that may make such conversion technologies economically competitive. Such R&D is performed at NETL in support of the Office of Fossil Energy and Carbon Management efforts to create value-added, carbon-derived products in conjunction with the reduction or elimination of CO_2 emissions. The tool was developed by SSAE researchers S. Hughes*, M. Turner*, D. Kauffman and G. Hackett.

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// HIGHLIGHTS cont'd

Techno-Economic Analysis of a SOFC and CAES Hybrid Carbon Conversion Concept Published

SSAE and the Idaho National Laboratory initiated a collaborative effort in 2018 to explore solid oxide fuel cell (SOFC)-based hybrid carbon conversion concepts to understand the potential of coupling SOFC with other electricity generating and/or storage technologies as part of an integrated energy system. After initial scoping and screening studies were completed, SSAE researchers focused on a hybrid system consisting of SOFC and compressed air energy storage (CAES), as it was determined that this system had the potential to be a flexible, low-carbon (with carbon capture) solution to an electrical grid with increasing amounts of fluctuating variable renewable energy, depicted in the block flow diagram, Figure 3.

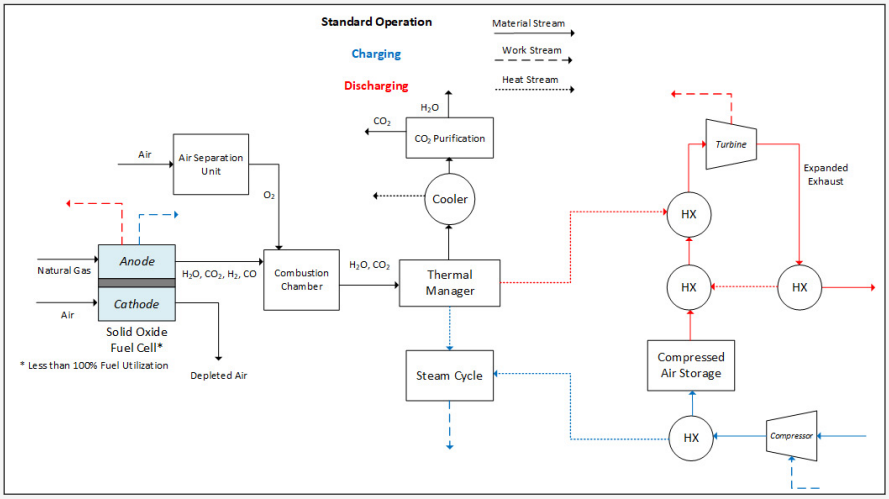

Figure 3. Block Flow Diagram of Hybrid SOFC and CAES System

Through performance modelling, SSAE researchers, K. Bucheit*, A. Noring*, A. Iyengar* and G. Hackett, discovered that a ratio of 3.1 for SOFC to CAES power scale for thermal integration eliminates the need of compressed air reheat which is typically done with natural gas burners. The theoretical hybrid system is cost competitive with NGCC power plants with carbon capture when normalized to a similar power output and can be further improved when integrated into a cheaper electricity market. The resulting report Techno-Economic Analysis of a Thermally Integrated Solid Oxide Fuel Cell and Compressed Air Energy Storage Hybrid System has been published in energies.

Staff Spotlight

Daison Yancy Caballero has been contributing to the SSAE's Process Systems Engineering Research Team's efforts in modeling, optimization, and conceptual design of advanced energy systems, point-source carbon capture, and direct air CO_2 capture technologies, since joining NETL in 2020 as a site support contractor. He has played a key role in projects such as Carbon Capture Simulation for Industrial Impact (CCSI^2), Carbon Dioxide Removal (CDR), and EXXON-DAC.

In these projects, he has contributed to the development of mathematical models, process optimization, and conducted techno-economic analyses for various carbon capture and direct air capture process energy systems.

Daison was born in La Guajira, Colombia, and holds a bachelor's degree in chemical engineering (2009) from the Industrial University of Santander, Colombia. He pursued advanced studies in chemical engineering in Brazil, earning a master's degree (2012) and a Ph.D. (2016) from the University of Campinas. During his doctoral studies he served as a visiting research scholar, collaborating with Lorenz Biegler, the Covestro University Professor of Chemical Engineering at Carnegie Mellon University, on the development of optimization strategies to enhance gas-solid chemical reactor design. Subsequently, as a postdoctoral research associate at the Brazilian Bioethanol Science and Technology Laboratory in Campinas, Brazil, he focused on computational fluid dynamics (CFD) models for flow and heat modeling in porous media. Later, at Northwestern University in Evanston, IL, he worked on developing an optimization framework for integrating the design of metal-organic framework (MOF) materials and adsorption processes for carbon capture applications. Daison is enthusiastic about continuing his support for NETL in diverse energy-related projects.

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// NOTICES

Figure 4. PARETO Team held a Workshop at the New Mexico Produced Water Research Consortium Annual Meeting

PARETO Team Holds Workshop at the New Mexico Produced Water Research Consortium Annual Meeting

The team for Project PARETO—DOE's produced water optimization initiative—prepared and presented a workshop at the New Mexico Produced Water Research Consortium's (NMPWRC) annual meeting in Albuquerque, New Mexico in December 2023. The workshop attracted attendees from across the produced water community, including industrial practitioners, government and regulatory agencies, and academic researchers, Figure 4. The NMPWRC meeting featured presentations on topics such as produced water treatment technologies, produced water characterization and monitoring tools, and updates from the New Mexico Environment Department on proposed legislation in the state.

SSAE's PARETO team (Markus Drouven, Travis Arnold, Elmira Shamlou*, and Melody Shellman) presented the workshop to PARETO users. Approximately twenty participants took part in the workshop. Attendees benefited from a hands-on-keyboard and interactive experience in using PARETO software to model, analyze, and optimize produced water networks for on-shore oil and gas operations. Workshop participants learned how to:

- Input data into PARETO's graphical user interface.
- Represent a produced water network model.
- Run optimization algorithms to obtain the optimal water management and infrastructure buildout decisions.
- Perform sensitivity analyses for a variety of realistic scenarios, such as (a) seismic response area restrictions on saltwater disposal wells, and (b) availability of downstream beneficial reuse options for treated produced water.
- Analyze, interpret, and compare optimization results using GUI features.

PARETO's source code is available on GitHub, the graphical user interface is available for download as open-source software, and framework documentation is also available online. The workshop materials will be available as video tutorials soon.

Want to learn more about SSAE's work?

Click here to see previous SSAE newsletter issues

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// PERSPECTIVES

SSAE's Role in NETL's New National Methane Emissions Reduction Initiative (NEMRI)

Methane emissions are well known to contribute significantly to climate change. Despite its shorter atmospheric lifespan compared to carbon dioxide, methane is a highly potent greenhouse gas (GHG), with a 100-year warming potential 28 times that of carbon dioxide. According to the EPA, about one-third of current GHG-induced warming is attributed to anthropogenic methane emissions, with oil and natural gas operations identified as the foremost industrial source of methane emissions across the nation.

The majority of oil and gas production sites in the United States (roughly 80%) are low-production well sites yielding, on average, 15 barrels of oil equivalent per day or less. Despite contributing to only 6% of overall oil and gas production across the country, the combined emissions from these well sites constitute about 50% of the total methane emissions from all oil and gas production sites in the United States.[‡] Relative to their energy output, these well sites emit a disproportionate amount of methane, which makes them a particularly attractive target for environmental mitigation.

The 2022 Inflation Reduction Act provided EPA with over $1 billion to reduce methane emissions across the oil and gas industry under the Methane Emissions Reduction Program (MERP). In June of 2023, EPA and DOE announced an interagency partnership to jointly tackle the emissions mitigation challenge laid out by the MERP, with an initial emphasis on low-producing, so-called "marginal conventional wells".[†] The agreement included NETL, which has extensive experience in quantifying and reducing methane emissions from oil and gas operations. In particular, NETL agreed to manage a grant program that would provide up to $350 million in financial assistance to eligible states for mitigating methane emissions from marginal wells by permanently plugging these on a voluntary basis. In addition, NETL's Research and Innovation Center (RIC) was tasked with providing direct technical assistance to organizations across the emissions mitigation community participating in the MERP. In support of these efforts, NETL launched the **National Methane Emissions Reduction Initiative (NEMRI)**, Figure 5. NEMRI is composed of a multi-disciplinary team of researchers and technology experts from across NETL's RIC Directorates, including Geological & Environmental Systems (GES), Materials Engineering and Manufacturing (MEM) and Strategic Systems Analysis & Engineering (SSAE). Across all three divisions, NETL has extensive experience in developing technology solutions that contribute to a reduction in emissions from oil and gas infrastructure. NEMRI is designed to support both phases of the MERP, targeting emissions from marginal wells first, and addressing oil and gas emissions broadly thereafter.

The initiative is expected to provide tangible support to the emissions mitigation community in several ways: (1) developing open access online databases on marginal wells and other oil and gas infrastructure, (2) aggregating and processing available compliance/inspection reporting data on oil and gas infrastructure to predict the likelihood of methane leaks, (3) conducting field surveys and monitoring campaigns to better understand and predict the relationship between fugitive and episodic emissions, (4) designing and testing emissions monitoring approaches, (5) characterizing and improving plugging materials and processes, (6) developing and demonstrating advanced sensor technologies at scale, and (7) exploring novel emissions mitigation technologies that do not require outright plugging of wells or costly equipment upgrades. In addition, NEMRI is making NETL resources and technology experts available to provide on-demand technical assistance to the broader emissions mitigation community in support of the MERP.

[‡] Omara, M., Zavala-Araiza, D., Lyon, D.R., Hmiel, B., Roberts, K.A., and Hamburg, S.P. Methane emissions from US low production oil and natural gas well sites, *Nature Communications*, 2022 (13: 2085). https://doi.org/10.1038/s41467-022-29709-3

[†] EPA and DOE Announce Partnership to Provide More than $1 Billion to Reduce Methane Emissions from Oil and Gas Sector

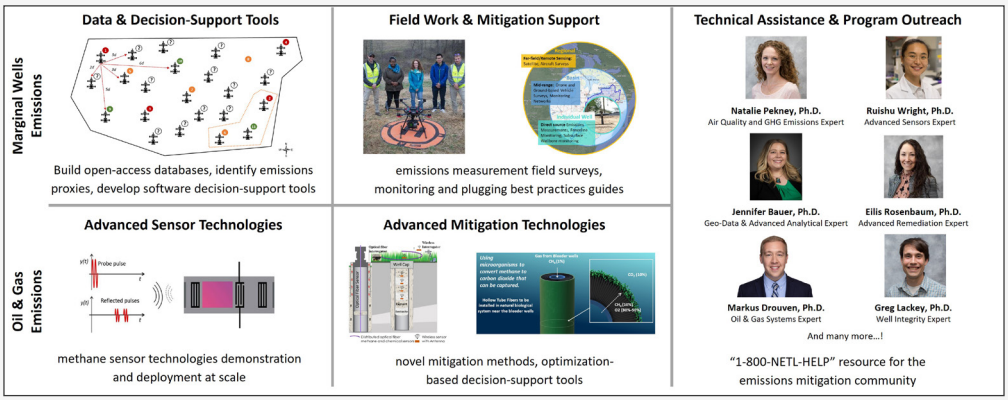

Figure 5. Overview of NETL's National Methane Emissions Reduction Initiative (NEMRI)

SSAE is expected to play a central role under NEMRI by developing and releasing optimization-based emissions mitigation decision-support software to help states and other MERP stakeholders identify, characterize, prioritize, and mitigate emissions from oil and gas operations. Specifically, with respect to the initial focus on marginal wells, SSAE's Process Systems Engineering (PSE) team is actively working with state regulators on a user-friendly software tool, tentatively referred to as PRIMO, that makes recommendations about (1) which wells to target for plugging campaigns (e.g., low-producing yet top-emitting wells that disproportionately affect disadvantaged communities), (2)

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// PERSPECTIVES (cont'd)

how to make efficient use of emissions quantification and well inspection resources, and ultimately (3) how to design and execute effective plugging and abandonment (P&A) campaigns. Figure 6 summarizes some of the key challenges and aspects related to the plugging and abandonment of marginal wells from a systems perspective.

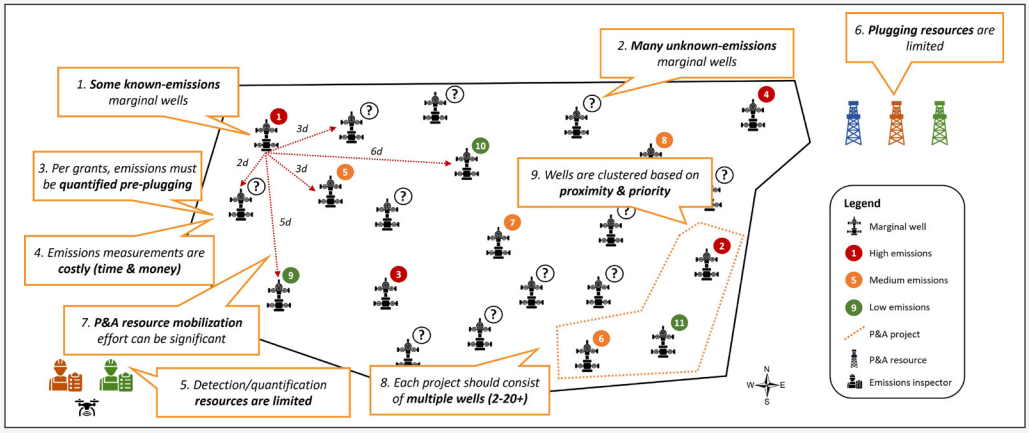

Figure 6 Challenges associated with P&A of marginal conventional wells

In developing MERP-specific emissions mitigation decision-support tools, SSAE's PSE team is leveraging decades of experience—and actual code architecture—from past and current NETL software frameworks, such as IDAES, CCSI, PARETO, and WaterTAP. Ultimately, the released software tools will (1) read in relevant data (e.g., location/characteristics of marginal wells, known/expected emissions profiles, availability of emissions quantification and P&A resources, mitigation campaign budget, etc.), (2) give users the ability to specify which objectives or constraints they wish to consider (e.g., maximize emissions reductions and/or minimize mitigation campaign costs subject to resource or staff shortages), and (3) return specific, actionable recommendations on where to focus efforts (e.g., wells, pipelines, compressors, etc.) and how to conduct efficient and effective emissions mitigation campaigns. As such, the capabilities developed by SSAE leverage and integrate the data, insights, and best practices established through NEMRI across NETL's multidisciplinary team—which is ultimately expected to benefit the broader emissions mitigation community.

// UPCOMING CONFERENCES AND EVENTS

SSAE federal staff and NETL support contractor personnel will attend or present at the following conferences February 2024:

- 48th International Conference and Expo on Advanced Ceramics and Composites
  The American Ceramic Society
  Participant: Jian Liu
  Daytona Beach, FL, January 28–February 2, 2024
- Energy Transition Summit: Grid Modernization Initiative and Clean Energy Cybersecurity
  Department of Energy
  Participants: Peter Balash, Alicia Dalton-TIngler, Kirk LaBarbara
  Arlington, VA, February 5–8, 2024
- New Waters: The Next Generation of Produced Water Management
  34th Annual Conference, Produced Water Society
  Presenters: Marcus Drouven, Miguel Zamarripa-Perez
  Houston, TX, February 6–8, 2024
- Joint DOE-DOI Technical Workshop on Basin Scale Issues for Carbon Storage
  Department of Energy and Department of the Interior
  Presenter: Robert Dilmore
  Reston, VA, February 13–14, 2024
- International Workshop Agreement (IWA) Sustainable Critical Minerals Supply Chains Workshop
  JAPAN Institute of Industrial Science
  Participants: Michelle Krynock, Tom Tarka
  Tokyo, Japan, February 15–16, 2024
- 2024 JISEA Annual Meeting (JAM24)
  Joint Institute for Strategic Energy Analysis (JISEA)
  Participant: Peter Balash
  National Renewable Energy Laboratory
  Golden CO, February 26–27, 2024

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UPCOMING CONFERENCES AND EVENTS (cont'd)

- 8th International Supercritical CO_2 Power Cycles Symposium
  Presenter: Eric Liese
  San Antonio, Texas: February 26–29, 2024
- Hydrogen Infrastructure Priorities to Enable Deployment in High-Impact Sectors
  DOE Hydrogen and Fuel Cell Technologies Office
  Participant: Nathan Weiland
  Alexandria, VA, February 27–28, 2024
- Orphan, Abandoned, Idle, and Marginal Wells: Opportunities with Plugging, Repurposing, Carbon Credits, and More Workshop
  AAPG/Pittsburgh Petroleum Geology Societies
  Participant: Markus Drouven
  Cranberry Township, PA, February 27–28, 2024

RECENT PUBLICATIONS

Reports

- Choisser, A., Mark-Moser, M., Mulhern, J., and Rose, K., Scoping Review of Global Offshore Geologic Carbon Storage Activities, DOE/NETL-2024/4798, NETL Technical Report Series, National Energy Technology Laboratory, Albany, OR, December 5, 2023.
- Wendt, A., Basista. E., Lin, S., Shih, C., Milligan, M., and Grant, T., Assessment of Water Management and Costs on CO_2 Geologic Storage Operations in Saline-Bearing Formations, National Energy Technology Laboratory, Pittsburgh, PA, July 28, 2023.

Presentations and Posters

- Mark-Moser, M., Mulhern, J., Choisser, A., and Rose, K., Global inventory and meta-analysis of offshore geologic carbon storage efforts. American Geophysical Union (AGU) Fall Meeting 2023, December 11–15, 2023, San Francisco, California. Poster Presentation.
- Mark-Moser, M., Creason, C.G., Mulhern, J.S., Shay, J., and Rose, K., Multi-factor assessment for decarbonization via technically viable carbon storage. American Geophysical Union (AGU) Fall Meeting 2023, December 11–15, 2023, San Francisco, CA.
- Morgan, D., Overview of the FECM/NETL CO_2 Saline Storage Cost Model (CO2_S_COM). USAE Saline Storage Cost Modeling Workshop, Washington, DC, December 12, 2023.
- Brewer, J., Dispatch Informed Hydrogen Production. DOE/NETL-2023/3929. USAEE 40th Annual Meeting, November 6–8, 2023, Chicago, IL.
- **Models/Tools/Databases**
- Industrial CO_2 Capture Retrofit Database (IND CCRD), DOE/NETL-2024/4408, Hughes, S., et al. December 20, 2023.
- NETL Electrochemical Conversion of CO_2 Sensitivity Analysis Tool, DOE/NETL-2024/4405, Hughes, S., Turner, M., Woods, M., Carr, S., Kauffman, D., and Hackett, G., December 15, 2023.
- Sensitivity Analysis Tool for Electrochemical Conversion of CO_2 to CO: User Guide, DOE/NETL-2024/4405, Hughes, S., Turner, M., Woods, M., Carr, S., Kauffman, D., and Hackett, G., December 15, 2023.

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// REFERENCE SECTION

Models / Tools / Databases

Carbon Capture Simulation Initiative (CCSI) Toolset

FECM/NETL CO_2 Transport Cost Model

FE/NETL CO_2 Saline Storage Cost Model

FE/NETL CO_2 Prophet Model

FE/NETL Onshore CO_2 EOR Cost Model

FECM/NETL Unconventional Shale Well Economic Model

Life Cycle Analysis Models

NETL CO2U LCA Guidance Toolkit

NETL UPGrants LCA Guidance Toolkit

IDAES Integrated Platform

IDAES Power Generation Model Library

Pulverized Coal Carbon Capture Retrofit Database (CCRD)

Natural Gas Combined Cycle CCRD

Industrial Sources CCRD

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Cost of Capturing CO_2 from Industrial Sources

Quality Guidelines for Energy System Studies

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