SSAE Newsletter

MAY // 2022 VOLUME 2.5

// 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

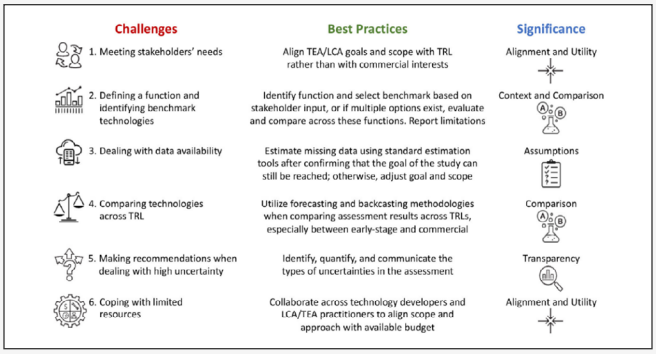
SSAE Researcher Contributes to Harmonized Framework for Environmental and Economic Assessments

Two articles presenting a common framework for conducting and reporting on life cycle assessment and techno-economic analysis (TEA) of emerging carbon capture and utilization (CCU) technologies were recently published in *Frontiers in Climate*. Life cycle assessment and TEA are methods for evaluating and quantifying environmental and economic opportunities and associated risks of product systems.

In the first paper, **Sheikh Moni*** and co-authors explained challenges to and best practices for identifying technology readiness levels (TRL) and conducting life cycle assessment and TEA of early-stage CCU technologies as outlined in the figure below. The second paper by Moni and co-authors described a method incorporating technology learning curves to forecast environmental performance and cost of CCU technologies at high adoption.

Moni completed these papers in collaboration with researchers in the International CCU Assessment Harmonization Group, which is part of the Global CO_2 Initiative (GCI) at the University of Michigan, which actively coordinates with NETL. GCI works with a broad range of research organizations and funding sources to advance research, development, and deployment of CCU technologies.

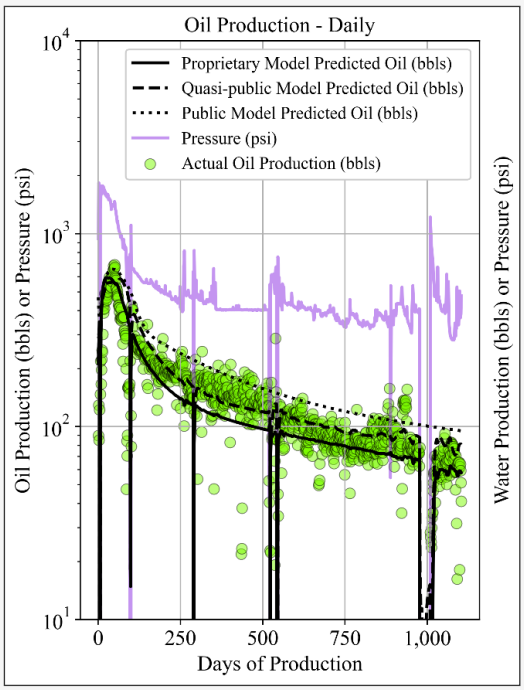
These papers are intended to help create consistent guidelines for assessing potential products from captured carbon dioxide (CO_2) and thereby advance the development and commercialization of CCU technologies.



Challenges to, best practices for, and significance of approaches in assessing emerging technologies

Report Evaluates Impact of Proprietary Data on ML Model Performance in Unconventional O&G Applications

SSAE recently released a report that evaluates the impact of proprietary data on the accuracy and utility of machine learning (ML) models. The goal of the study was to encourage broader data sharing to better study and understand areas where more extensive data might be needed (common to geoscience applications). The work involved an experimental study building ML models for a common unconventional oil and gas (O&G) time series production application but using different sets of well completion parameters – some largely relying on proprietary data and others on publicly available data. Model formulations evaluated included a Proprietary Model which contains an input feature set with data types that are predominantly proprietary in origin, a Quasi-public Model with a mix of inputs from proprietary and public origins, and a Public Model which consists entirely of data commonly available from public sources. The results demonstrate that certain data often kept proprietary (in this case well logs, production data at daily frequency, specific completion information at the stage-level resolution, and pressure data that provide a glimpse for how wells are operated) can substantially improve models (and ultimately understanding) for unconventional O&G production. The higher complexity models (Propriety Model and Quasi-public Model) that leverage proprietary data account for greater system variability and offer improved prediction accuracy. Additionally, these models can better account for transient well events, thereby approximating daily and cumulative production more effectively by improved handling of production irregularities (see example in figure below). Overall, the findings from this effort help pinpoint select data types that proved most insightful for generalizing production dynamics in a time-series fashion.



Daily oil production history for an interrupted well using the production prediction model variants

IDAES Version 1.13.0 Released

NETL's Institute for the Design of Advanced Energy Systems (IDAES) continues to advance SSAE's capabilities to design and optimize next-generation energy and process systems through the release of Version 1.13.0 of the IDAES Integrated Platform. Development of this new release was driven by the needs of several DOE projects in the areas of clean energy, hybrid energy systems, and water treatment technologies.

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// HIGHLIGHTS (cont'd)

One important new capability is integration with the open-source CoolProp package for pure component thermophysical property calculations, which can be combined with equations of state to simulate the properties of mixtures. The property correlations used by CoolProp were directly implemented within IDAES and combined with an interface for automatically retrieving parameters from CoolProp's extensive parameter database. Users need only identify the components of interest in their system for which they wish to use CoolProp, and the parameters and expression forms will be automatically loaded by the platform.

IDAES also recently announced the upcoming release of IDAES v2.0 for the end of 2022, which has been driven by the continued growth of projects using the toolset (both inside SSAE and externally).

SSAE Leads Submission to NAWI Pilot Project RFI

The advanced modeling capabilities within SSAE's IDAES and affiliated projects that can improve the effectiveness and efficiency of pilot-scale demonstrations were highlighted in a submission to the Pilot Program Request for Information (RFI) from the National Alliance for Water Innovation (NAWI). The capabilities include techno-economic modeling, dynamics, controls, uncertainty quantification, sequential design of experiments, and robust optimization. **Tim Bartholomew** led a team with SSAE researchers **Andrew Lee***, **Josh Morgan***, **Stephen Zitney**, **Anthony Burgard**, and **David Miller** and external collaborators from Carnegie Mellon University, the University of Notre Dame, and Lawrence Berkeley National Laboratory in this submission, which also emphasized that these capabilities could be integrated to WaterTap, a NAWI-funded water treatment techno-economic assessment tool that is being developed by the SSAE researchers.

Staff Spotlight

Since joining the Process and Cost Engineering Team last February, **Sarah Leptinsky*** advanced work under Pre-Combustion Capture, Existing Plant Improvements, and Multi-Program Support. She identified advanced hydrogen and CO_2 separation technologies for future analysis, updated post-combustion capture quotes in the forthcoming Cost and Performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity (Revision 4a) report, and is working on a biomass-based circulating fluidized bed boiler model to meet the demand for net-zero CO_2 emissions power generation.

Originally from the Pittsburgh area, Sarah graduated from the University of Pittsburgh with a B.S. in Chemical Engineering. She participated in a co-op at Underwriters Laboratory and volunteers at the Carnegie Science Center.

// NOTICES

NETL Adds Capabilities to WaterTAP

The development of WaterTAP (previously named ProteusLib), a water treatment process modeling tool, is being led by SSAE's **Tim Bartholomew**. This techno-economic assessment tool for existing and emerging water treatment technologies is based on the IDAES platform. WaterTAP development is funded by two sources: 1) the NAWI, DOE's desalination hub and 2) DOE FOA 0002336, Research and Development for Advanced Water Resource Recovery Systems. While both funding sources seek to develop water treatment models, each is focused on different TRLs and application areas. NAWI is focused on early-stage technologies (TRL 2-4) for desalination, and DOE FOA 0002336 is focused on more mature technologies up to the pilot demonstration (TRL 4-7) for wastewater treatment and resource recovery.

The most recent release in March 2022, WaterTAP Version 0.4.0, included initial models for evaporative desalination technologies (mechanical vapor compression and forced circulation crystallization) and several simple models for wastewater resource recovery technologies (e.g. solar evaporator, electrochemical nutrient removal, membrane bioreactor, anaerobic digester). The release also included the integration of more than 40 simple models spanning a wide range of water treatment technologies from another previous NAWI modeling effort called WaterTAP[3].

// NOTICES (cont'd)

DOE's Produced Water Optimization Initiative Presented to Federal Water Treatment Interagency Working Group Committees

In March 2022, **Markus Drouven** was twice invited to speak on DOE's Produced Water Optimization Initiative, "Project PARETO," to Federal Water Treatment Interagency Working Group committees. Among other topics, the working group is concerned with concentrate and residuals management, as well as water reuse and produced water opportunities. The committees involved representatives from several federal agencies and other organizations including the U.S. Department of Agriculture, National Aeronautics and Space Administration, U.S. Army Corps of Engineers, U.S. Bureau of Reclamation, U.S. Environmental Protection Agency (EPA), U.S. Geological Survey, U.S. Military Academy at West Point, U.S. Navy, U.S. Army, and National Science Foundation.

I-WEST CO_2 Storage and Utilization Workshop Summary Released

As part of the Intermountain West Energy Sustainability & Transitions (I-WEST) initiative, a summary of findings and takeaways from an NETL SSAE-led workshop on CO_2 storage and utilization was released. The workshop targeted discussion of the role of CO_2 utilization and storage in achieving carbon neutrality in the Intermountain West by eliciting expert knowledge as presented by field practitioners currently leading CO_2 storage/utilization projects.

LCA Work at Various Conferences/Events

On April 20, 2022, life cycle analysis (LCA) at NETL was virtually presented by **Timothy Skone** at a training session, hosted by the American Center for Life Cycle Assessment (ACLCA), through the LCA Institute. The LCA Institute allows professionals the ability to learn from industry experts on the tools, resources, and strategies needed to apply LCA to sustainability efforts.

SSAE's LCA will be well represented at the 2022 International Symposium on Sustainable Systems and Technology (ISSST) to be held June 21–23, 2022 in Pittsburgh, PA. Work will be featured in various presentations either by or co-authored by SSAE researchers. Please see the links below for full author lists on these presentations. SSAE researchers will also participate in panels or chair sessions.

- ISSST Special Session: Life Cycle Assessment of Emerging Technologies: Update on the SETAC/ACLCA Working Group Progress by Joule Bergerson et al. for the Emerging Tech: Special Session: Life Cycle Assessment of Emerging Technologies session.
- The Potential for Bio-energy Projects to Achieve Negative Emissions by **Derrick Carlson*** et al. during the ISIR-Bio: Harnessing the Biosphere session.
- The Right Measure Data Quality Metric for Greenhouse Gas Emissions Accounting of U.S. Crude Oil by Cathy Crawford et al. in the poster session.
- Life Cycle Greenhouse Gas Emissions and Water Consumption from Existing and Emerging Hydrogen Pathways by **Megan Henriksen*** et al. and Life Cycle Analysis of Mineralization of Concrete Products for CO_2 Utilization by **Sheikh Moni*** et al. for the ISIR-Mat: Innovations in Materials session.
- Life Cycle Analysis of Emerging CO_2 Utilization Technologies: Challenges and Current Best Practices by **Sheikh Moni*** et al. in the ASAM-Circular2: Materials Resources Circularity 2 session.
- Natural Gas as a Decarbonization Strategy: Evaluating Emission Mitigation Opportunities throughout the Value Chain by **Katherine Mumm*** et al. during the ASAM-Energy2: Advances in sustainability assessment methods for Energy session.
- Land Use Change Modeling in Life Cycle Assessment at the National Energy Technology Laboratory by **Shirley Sam*** et al. for the ASAM-Bio: Bio-based Systems session.
- **Derrick Carlson*** will be part of the Lunch & Local Sustainability Panel, which will discuss the sustainability endeavors taking place in Pittsburgh, PA. He will also serve as a local host for the conference and one of the Student Presentation and Poster Competition Chairs for the poster session.
- **Timothy Skone** will be involved in a Career Panel that aims to introduce career paths in sustainability to ISSST student and post-doctoral participants.

// SSAE CORE CAPABILITIES

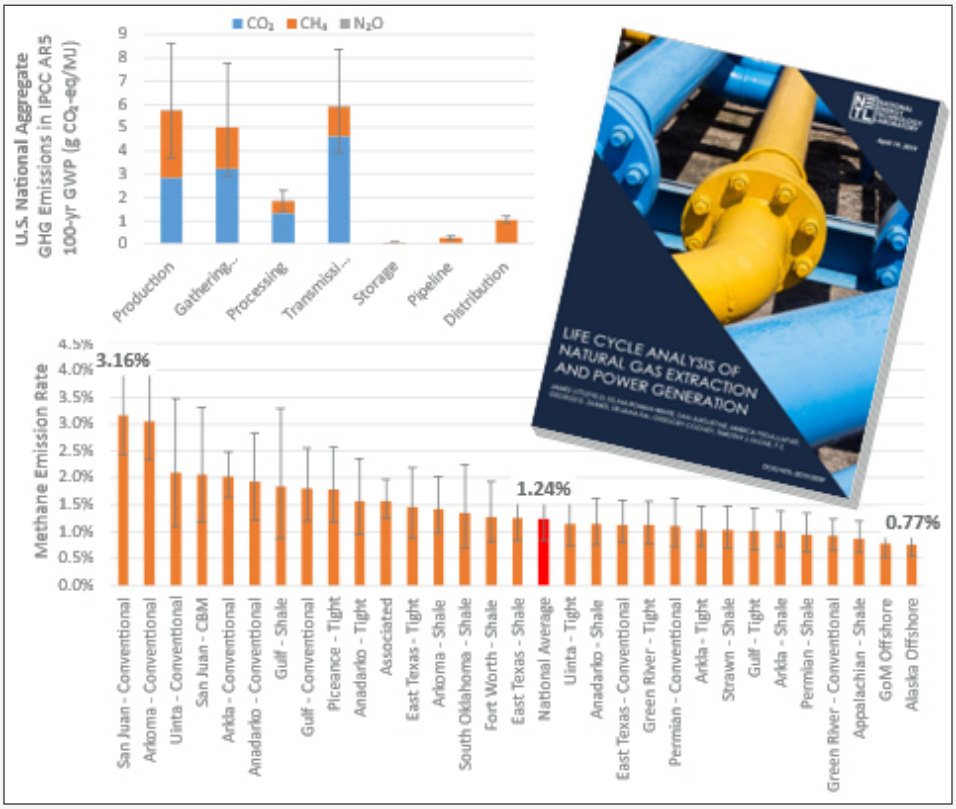
LCA at NETL

SSAE's Life Cycle Analysis (LCA) competency within the Energy Systems Analysis Team (ESAT) supports NETL's mission of driving innovation and delivering solutions for an environmentally sustainable future. The team provides LCA models, tools, and data that can be utilized to inform NETL about the environmental profile of potential research and development pathways and new and emerging technologies. At NETL, the LCA team creates transparent and unbiased cradle-to-grave models in support of federal energy research decisions and to inform policy makers. Open source model development requires deep LCA expertise and industry-standard environmental assessment techniques with transparency and flexibility to model advanced technologies that could be deployed in complex and changing energy futures. The team's work has recognized NETL as a national and global leader on LCA as evidenced by the ACLCA Government LCA Leadership Award in 2017 and 2019.

SSAE's LCA team develops tools and models that respond to NETL leadership and DOE emergent requests. The LCA team developed the first-of-a-kind U.S. fossil energy (coal, natural gas, petroleum) and U.S. electricity baseline made in conjunction with the U.S. EPA. In addition, the team is evaluating geospatial effects of emissions releases by incorporating reduced-form air quality modeling using established platforms AP3, EASIUR, and InMAP. The team couples these platforms with LCA inventory data to create models with a deeper understanding of the localized impacts from PM2.5 emissions and its associated precursors.

LCA as generally practiced draws on knowledge, skills, and tools across domains and disciplines to provide a quantitative assessment of a system's cradle-to-grave energy and environmental impact. Process-based LCA builds models for systems by connecting process building blocks (unit processes) that incorporate component- or facility-level data from industry, literature, and government. The unit processes are connected by material and energy flows, and the inputs and outputs within the system are summed to determine the total environmental impacts of products. Within this life cycle framework, NETL SSAE provides expertise in performing LCAs of energy products, including methane quantification from O&G; CO_2 capture, storage, and utilization; and electricity generation and fuel production national baselines.

The LCA team uses and creates datasets and models that support LCA of energy systems, providing unit processes and inventories to public databases such as the Federal LCA Commons and the NETL Unit Process Library. Data science, statistical techniques, and software enhanced by Python scripts are used to collect and analyze emissions and resource consumption data from a variety of large-scale repositories including the U.S. EPA's Greenhouse Gas Reporting Program (GHGRP), National Emissions Inventory (NEI), Toxics Release Inventory (TRI), and Air Markets Program Division (AMPD). The LCA team includes personnel who have supported U.S. EPA's development of these datasets for decades. This experience is leveraged to identify the right data for the question at hand. The emissions data are coupled with the activity information for the sector of interest using datasets such as Enverus (DrillingInfo) for the O&G sector to develop normalized emissions factors for use within the context of the LCA.



Life cycle models are developed in openLCA, an open-source life cycle software modeling platform, which provide system-wide environmental emissions and resource use. These emissions are translated into a comprehensive set of potential environmental impacts using the EPA Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) method, reduced-form air quality models to evaluate geospatial effects of emissions releases, the AWARE-US water stress model to incorporate localized water use impacts, and marginal abatement cost (MAC) to measure the scale and cost of emission reduction technology options.

// SSAE CORE CAPABILITIES (cont'd)

The environmental and climate impacts of new energy and carbon management technologies need to be quantified and compared to existing technologies to ensure that they represent improvements in environmental sustainability in alignment with NETL's mission. The NETL CO2U LCA Guidance Toolkit helps DOE Carbon Utilization Program project principal investigators meet LCA requirements, improve decision-making by ensuring consistency and transparency across Carbon Utilization Program projects, guide a wider audience outside the Carbon Utilization Program in conducting LCAs on carbon utilization (CO2U) systems, and advance the global discussion on CO2U LCA. CO2U can reduce GHG emissions by recycling waste CO_2 and transforming it into valuable products (e.g., synthetic fuels and carbon fibers) and applications (e.g., energy storage and enhanced resource recovery). The toolkit comprises the NETL CO2U LCA guidance document, openLCA life cycle inventory database, openLCA results contribution tool, LCA documentation spreadsheet, LCA report template, openLCA model training resources, and LCA subject matter expert support.

Work products are dependent on the needs of the client; therefore, LCA modeling and analysis needs to be tailored and fine-tuned to meet client needs each time. For instance, certain projects need quick turn-around streamlined LCAs in support of, for example, DOE's Loan Programs Office submissions that use a spreadsheet and produce only a presentation slide deck deliverable. Other projects need rigorous LCAs of current or emerging systems and result in custom openLCA models and large research reports. – Contributed by **Matthew Jamieson** and **Timothy Skone**, SSAE's ESAT

// UPCOMING

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

- 2022 IEEE-IAS/PCA Cement Conference
  Presenter: **Timothy Fout**
  Las Vegas, NV, May 1–5, 2022
- Offshore Technology Conference 2022
  Participants: **Timothy Grant** and **Luciane Cunha**
  Houston, TX, May 2–5, 2022
- FY22 FECM Spring R&D Project Review
  Presenters: **Eric Grol** – Overview of Emissions Control Research at NETL, **David Miller** – IDAES – Institute for the Design of Advanced Energy Systems, **Paul Myles*** – Evaluation of NGCC with Capture for Long Duration Energy Storage (LDES), and **Ivonne Pena-Cabra*** – Integration of Energy Storage in Fossil Energy Power Plants (ES-FE) Market Analysis
  Participants: **Eric Lewis**, **Robert Stevens**, and **Stephen Zitney**
  Virtual, May 2–12, 2022
- NAWI Alliance Spring Meeting 2022: Research Program Immersion
  Presenter: **Timothy Bartholomew**
  Virtual, May 3, 2022
- 51st Annual Eastern Fuel Buyers Conference: Challenge of Energy Transitions
  Participant: **Morgan Summers**
  Orlando, FL, May 4–6, 2022
- 2022 DUG Permian Basin & Eagle Ford Conference and Exhibition
  Participant: **Markus Drouven**
  Fort Worth, TX, May 16–18, 2022
- AISTech 2022
  Participant: **Timothy Fout**
  Pittsburgh, PA, May 16–18, 2022
- Electric Power Research Institute Water-Energy Transformation Forum
  Participant: **Eric Grol**
  Charlotte, NC, May 18–19, 2022
- CCU TEA and LCA Guidance – A Harmonized Approach Workshop
  Participants: **Samuel Henry***, **Michelle Krynock**, **Sheikh Moni***, and **Timothy Skone**
  Hybrid (Virtual and Ann Arbor, MI), May 18–20, 2022
- SPE Forum: The Role of Oil and Gas in Emerging Hydrogen Markets
  Presenter: **Robert Wallace***
  Denver, CO, May 22–26, 2022
- 2022 ARPA-E Energy Innovation Summit
  Participant: **John Brewer**
  Denver, CO, May 23–25, 2022

// CONFERENCES AND EVENTS

- 2022 IEEE-IAS/PCA Cement Conference
  Las Vegas, NV, May 1–5, 2022
- FY22 FECM Spring R&D Project Review
  Virtual, May 2–12, 2022
- NAWI Alliance Spring Meeting 2022: Research Program Immersion
  Virtual, May 3, 2022
- SPE Forum: The Role of Oil and Gas in Emerging Hydrogen Markets
  Denver, CO, May 22–26, 2022

// RECENT PUBLICATIONS

Articles/Manuscripts

- A. W. Zimmermann, T. Langhorst, **S. Moni***, J. A. Schaidle, F. Bensebaa, and A. Bardow, "Life-Cycle and Techno-Economic Assessment of Early-Stage Carbon Capture and Utilization Technologies – A Discussion of Current Challenges and Best Practices," *Frontiers in Climate*, March 28, 2022.
- G. Faber, A. Ruttinger, T. Strunge, T. Langhorst, A. Zimmerman, M. van der Hulst, **S. Moni***, F. Bensebaa, and L. Tao, "Adapting Technology Learning Curves for Prospective Techno-Economic and Life Cycle Assessments of Emerging Carbon Capture and Utilization Pathways," *Frontiers in Climate*, April 14, 2022.
- X. Gao, B. Knueven, J. D. Siirola, **D. C. Miller**, and A. W. Dowling*, "Multiscale simulation of integrated energy system and electricity market interactions," *Applied Energy*, vol. 316, article 119017, 2022.

Reports

- A. Wendt, E. Basista, **N. Pastorek***, G. Lackey*, **D. Vikara***, and **T. Grant**, "Cost Impacts of Risk-Based Methods for Defining AoR and PISC Duration of a CO_2 Storage Project Through NRAP Tools and FE/NETL CO_2 Saline Storage Cost Model," National Energy Technology Laboratory, DOE/NETL-2022/3245, Pittsburgh, PA, March 31, 2022.
- **E. Lewis**, **S. McNaul***, **M. Jamieson**, **M. Henriksen***, **H. S. Matthews***, **J. White***, L. Walsh, J. Grove, **T. Shultz**, **T. Skone**, and **R. Stevens**, "Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies," National Energy Technology Laboratory, DOE/NETL-2022/3241, Pittsburgh, PA, April 12, 2022.

Conference Proceedings and Events

- **M. Jamieson** and **T. Skone**, "Life Cycle Analyses of Point Source Carbon Capture and CO_2 Destinations at the National Energy Technology Laboratory," presentation at the Conference on Innovations in Climate Resilience, Columbus, OH, March 30, 2022.
- **K. Bello***, **D. Vikara***, D. Remson, and **D. Morgan**, "Dimensionally Reduced Model for Rapid and Accurate Prediction of Gas Saturation, Pressure, and Brine Production in a CO_2 Storage Application: Case Study at the SACROC Field," presentation at the AAPG Carbon Capture, Utilization, and Storage Conference, Houston, TX, March 31, 2022.
- **N. Wijaya***, **D. Vikara***, **D. Morgan**, **T. Grant**, and D. Remson, "Basin Management of Geologic CO_2 Storage: Effect of Well Spacing on CO_2 Plume and Pressure Interference," paper presented at the 2022 SPE Western Regional Meeting, Bakersfield, CA, April 26, 2022.

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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

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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