SSAE Newsletter

MARCH // 2022 VOLUME 2.3

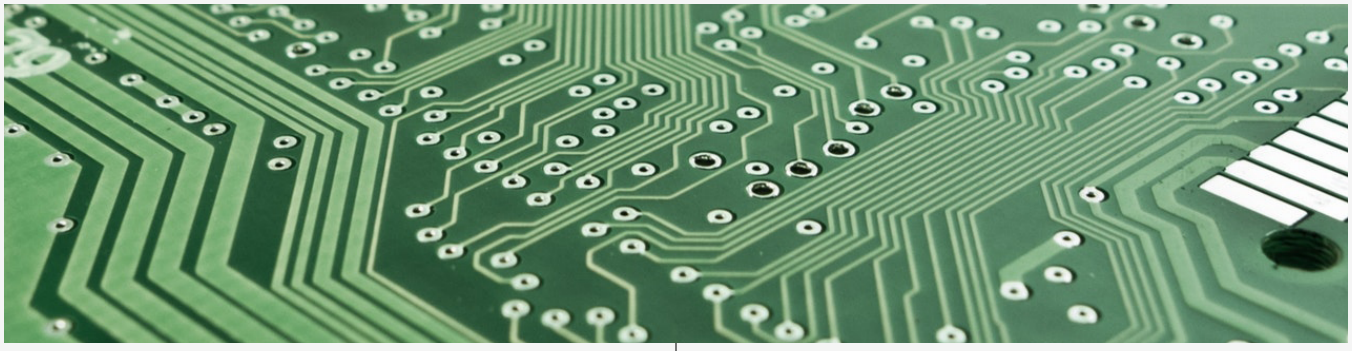
// ABOUT

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



High Carbon Capture Rate Cost Estimates are Focus of New Report

Cost and performance estimates for F-class natural gas combined cycle (NGCC) and conventional supercritical pulverized coal power plants equipped with post-combustion carbon capture systems designed for capture rates greater than 90% was discussed in a recent report by Alexander Zoelle, **Tommy Schmitt***, **Sally Homsy***, **Mark Woods***, **Travis Shultz**, **Timothy Fout** and Jeffrey Hoffmann. This report helps fill an urgent need for credible analyses that provide insight into deep-decarbonization options for electricity generating systems with greater than 90% capture. The report is an interim update to NETL's "Cost and Performance Baseline for Fossil Energy Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity" (Revision 4), which is in the process of being revised.

New CO2U Guidance Toolkit Debuts

Version 2 of the NETL CO2U LCA Guidance Toolkit was recently released. Since its initial release in 2019, major changes have been made to the toolkit including updated guidelines to reflect new carbon dioxide (CO_2) sources with industrial capture and direct air capture (DAC) as well as new guidelines for the inclusion of land use change impact.

The NETL CO2U LCA Guidance Toolkit is meant to help DOE Carbon Utilization Program project principal investigators meet life cycle analysis (LCA) requirements and improve decision-making, guide a wider audience in conducting LCAs on carbon utilization (CO2U) systems and advance the global discussion on CO2U LCA.

NETL Advances FLECCS Project

NETL, in collaboration with Susteon, Svante and the Los Angeles Department of Water and Power, is evaluating a rapid cycle thermal swing adsorption CO_2 capture technology under the Advanced Research Projects Agency-Energy's (ARPA-E) FLExible Carbon Capture and Storage (FLECCS) program. Phase 1 of this project, scheduled to end in March 2022, involves designing a flexible capture system that maximizes the net present value (NPV) for a power generator operating in a high variable renewable energy grid with carbon prices of $100–$300/ton. A quarterly update was given to ARPA-E that included results from the NPV optimization for 14 different sets of locational marginal prices (LMP) for an entire year and three different carbon tax prices. The analysis required formulating and solving a two-stage stochastic mixed integer non-linear programming problem to identify the optimal design and operation simultaneously. The project is on track for Phase 2 which will include pilot testing and analyzing system operation in real-time.

NETL has developed a unique capability to optimally design and operate capture systems that are flexible under varying price and operating scenarios as part of this effort. This research will help accelerate development of flexible carbon capture technologies, which will be a critical component for a decarbonized grid.

NETL Collaboration Paves Way for Integrated DAC Systems

The advanced optimization capabilities of SSAE's Process Systems Engineering Research Team were used to reduce cost of CO_2 removal technologies in work with Exxon Mobil Research and Engineering Company to assess integrating DAC systems with NGCC to achieve net-zero emissions. The objective was to develop an optimization framework for net-zero emissions on an NGCC power plant by combining a conventional post-combustion capture system using a second-generation solvent with adsorbents for low concentration CO_2 streams. This optimization framework was developed using the Institute for the Design of Advanced Energy Systems (IDAES) integrated platform. Phase 1 demonstrated the optimal design of adsorbent beds using a conventional sorbent while minimizing the overall cost of the system. In Phase 2, the team will screen high performing sorbents for DAC and evaluate the potential of advanced reactor configurations.

IDAES Demonstrates ML-Augmented Flexibility Analysis

NETL's IDAES demonstrated the use of machine learning (ML) to augment the flexibility analysis of integrated energy systems. By using neural network-based decision rules, the feasibility of operation of a given system design can be analyzed for many uncertain parameters. The ML-based flexibility analysis removes the inner minimization problem and reduces the overall optimization problem from a nested bi-level optimization to a single-level optimization problem. The IDAES flexibility analysis module now enables the computational solution of flexibility problems with sampling, vertex enumeration, active constraint strategy and decision rules. Planned next steps include analyzing the flexibility of a solvent-based carbon capture system model under development for use as a standard IDAES uncertainty quantification test problem.

* NETL Support Contractor

// NOTICES

NETL Invests in National LCA Capability

Scott Matthews* and Ben Young* led a first-of-its kind internal training to expand analysis capabilities within the NETL LCA Team. The LCA Team completed training sessions on life cycle thinking (e.g., history of LCA and quantitative methods) and environmental assessment (e.g., environmentally extended input-output models and life cycle impact assessment) and openLCA software features (e.g., uncertainty analysis and flow mapping) for performing LCA. With the Infrastructure Investment and Jobs Act recently passed into law, this training comes at a time when energy investment and decarbonization goals demand NETL's expertise and capabilities in LCA.

CESAR1 Work Featured at UTCCS-6

By invitation, a CESAR1 solvent system process model for carbon capture applications developed with Norway's Technology Centre Mongstad was presented by the Carbon Capture Simulation for Industry Impact ($CCSI^2$) team at the University of Texas 6th Conference on Carbon Capture and Storage (UTCCS-6) in January 2022. CESAR1 is a proposed alternative to the baseline aqueous monoethanolamine system for amine-based carbon capture. The model will be released as part of the open-source Carbon Capture Simulation Initiative (CCSI) Toolset in the near future.

SSAE Research and CCTS Highlighted at Produced Water Society Seminar

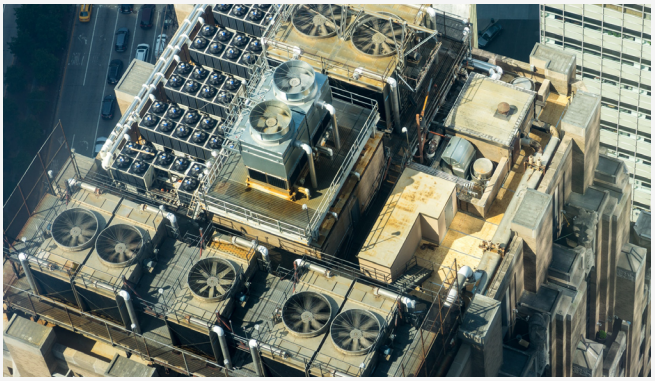
SSAE researchers presented at the 2022 Produced Water Society Seminar in February 2022:

- NETL's collaboration with Olympus Energy to optimize produced water management in the Appalachian Basin was presented by **Markus Drouven** and Olympus Energy Chief Operating Officer Michael Wahl. The goal of this ongoing collaboration is to explore opportunities for leveraging cutting-edge mathematical optimization technology to i) minimize community impacts of water management, ii) increase produced water reuse, iii) reduce trucking activity, and iv) decrease costs associated with produced water management. The partnership is part of the U.S. DOE Office of Fossil Energy and Carbon Management's (FECM) Produced Water Application for Beneficial Reuse, Environmental Impact and Treatment Optimization (PARETO) initiative. Based on recent case studies conducted by NETL's project team and Olympus Energy, this joint talk showcased PARETO's capabilities to optimize the coordination of i) produced water deliveries, ii) freshwater sourcing, iii) injection and/or treatment volumes, and iv) utilization, placement and sizing of temporary water storage facilities – all while meeting the completions water demand and satisfying regulatory, logistical and operational constraints.
- An overview of the current capabilities of PARETO, a cutting-edge, open-source decision-support platform that helps organizations leverage advanced mathematical optimization techniques to support daily operations and design mid- and long-term strategic plans for produced water management, was discussed in a presentation co-authored by **Andres Calderon*** and **Miguel Zamarripa-Perez***. This presentation showcased how PARETO can be implemented to deploy produced water infrastructure while reducing operational costs and realizing environmental benefits in terms of water reuse. This work was motivated by feedback from PARETO's stakeholder board to ensure that PARETO responds to the pressing challenges of the produced water community. The presentation was well received by the produced water community and has been highlighted by one of the organizations that attended the seminar in a recent news release.

A Carbon Capture, Transport and Storage (CCTS) Workshop was also held during this seminar to familiarize the produced water community with the fundamentals of CCS and to highlight specific opportunities for the community to become involved in CCTS efforts leveraging existing infrastructure and expertise. SSAE's **David Miller** and **Markus Drouven** presented in this workshop along with Dustin Crandall (NETL) and Lisa Henthorne (DOE-Lawrence Berkeley National Laboratory [LBNL]). John Litynski (DOE-HQ) provided an introduction and stressed the importance of CCTS research within DOE's portfolio. The workshop was organized by **Markus Drouven** at the request of Project PARETO's stakeholder board.

Optimal Design of Product Families to be Featured at PSE 2021+

A method of designing heating, ventilation and air conditioning products given system requirements and a set of off-the-shelf components will be discussed in a paper, "Optimization-based Design of Product Families with Common Components," that was accepted for presentation at the 14th International Symposium on Process Systems Engineering (PSE 2021+) in June 2022. The IDAES integrated platform was used for modeling and optimization in this collaboration between NETL, Carrier Global Corporation, The University of Minnesota, Carnegie Mellon University and Sandia National Laboratories. Applications of interest to NETL include design of modular energy systems where standardized components can be used to build modular systems of various capacities.

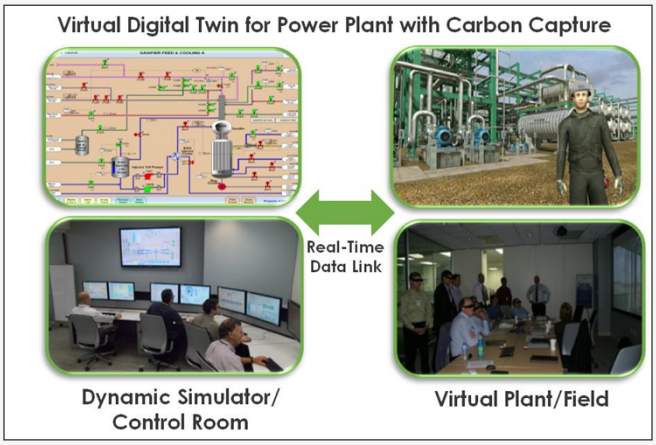


// NOTICES (cont'd)

SSAE Researcher Highlights RL-Based Controls for Flexible Operation of Applied Energy Systems

SSAE research on ML-based control for the flexible operation of applied energy systems was highlighted by **Stephen Zitney** at NETL's Science-Based Artificial Intelligence and Machine Learning Institute (SAMI) Artificial Intelligence for Applied Energy Day (AI4AE) workshop in January 2022. The presentation described a novel application of reinforcement learning (RL) for online dynamic tuning of model predictive controllers (MPC) for flexible operations. Dynamic simulation results showed that the RL-MPCs reduce environmental emissions and treatment costs during load-following operation through learning and implementation on a first-principles nonlinear dynamic model validated using industrial operating data. The interactive workshop focused on building awareness of crosscutting artificial intelligence/ML efforts, learning about NETL and FECM research on these emerging topics and promoting knowledge sharing across the research and development (R&D) community.

SSAE Researcher Delivers SMART Initiative Webinar on Virtual Digital Twins



The use of virtual digital twins for research, training and education on mitigating the negative impacts of flexible operations on plant performance, health and emissions was discussed by **Stephen Zitney** in January 2022 for a DOE Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) Initiative webinar. The presentation highlighted the development, testing and deployment of virtual power plant digital twins combining real-time high-fidelity dynamic simulators with ML-based hybrid models for control room operations with immersive virtual reality-based plant walkthrough environments for field operations. Virtual digital twins serve as test beds to help address the critical R&D, workforce training and education challenges facing the power industry on its drive toward cleaner, more flexible plant operations. NETL's IDAES was also highlighted for developing first-principles dynamics, control and health models, as well as ML-based surrogate models, that can be used to optimize the flexible design and operation of integrated energy systems with grid/market dynamics. The SMART Initiative is a ten-year, multi-organizational effort that is transforming understanding of the subsurface through application of science-based ML and data analytics, real-time visualization, forecasting and virtual learning. Funded by DOE's Carbon Storage and Upstream Oil & Gas programs, the SMART Visualization Platform Prize Challenge is creating a new, intuitive data visualization tool for the subsurface environment that can be readily accessible by scientists, engineers, subsurface operators and other decision-makers.

H_2 Baseline Pending Publication

SSAE is finalizing the "Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies" (H_2 Baseline) report – an independent assessment of the cost and performance of six hydrogen (H_2) production plant configurations. Levelized cost of hydrogen, in real 2018 dollars, is the main figure of merit of the report, and the CO_2 capture strategy employed for each case recovers greater than 90% of the carbon entering the plant boundary. Reporting methodology is consistent with NETL's 2019 revisions to their Quality Guidelines for Energy System Studies (QGESS) and Revision 4 of their Bituminous Baseline Report. Attributional global warming potential profiles of the impactful energy and material streams entering and exiting the plant boundaries were used to develop life cycle greenhouse gas emissions results for each case and are expressed as CO_2 equivalents on a cradle-to-gate basis. In addition to informing technology comparisons, the reference plant configurations found in this report provide perspective for regulators and policy makers. From an R&D perspective, this report may be used to assess goals and metrics and to provide a consistent basis for comparing developing technologies.

SSAE Welcomes Michelle Krynock

Michelle Krynock is joining SSAE's Energy Systems Analysis Team. As an NETL site support contractor for the last six years, Michelle performed life cycle analyses across technological areas such as carbon capture, utilization and storage as well as coal and natural gas production. Michelle also contributes to collaborative working groups such as the Federal LCA Commons Working group and the International CCU Assessment Harmonization. Michelle holds a bachelor's degree in civil and environmental engineering as well as engineering and public policy from Carnegie Mellon University. In her free time, Michelle enjoys reading, watching and writing fiction and is raising two cats with her partner.

// PERSPECTIVES

Effect of 2021 Winter Storm Uri on ERCOT and Potential Improvements

Between February 13–17, 2021, Winter Storm Uri drove through the central United States and created a deep freeze throughout the state of Texas which led to electricity outages, natural gas shortages, 246 deaths [1] across 77 counties in the state and an estimated economic toll between $80–$130 billion [2]. The collapse of the generation grid operated by the Electric Reliability Council of Texas (ERCOT), the electric grid operator that manages over 75% of Texas, was due to a combination of lack of preparedness by both the utility and natural gas sectors, and an already high percentage of generators offline due to maintenance. The freeze caused many generating units—across fuel types—to trip offline and become unavailable. This included the freezing of wind turbines and wind generation operating at one-seventh of its installed capacity. Almost 10,000 megawatts (MW) of generation was lost due to sub-freezing, and about 10,500 MW of customer load was shed at the highest point. This is enough power to serve approximately two million homes. From February 14–20, 2021, approximately 69% of Texas residents were without electricity and 49% were without running water [2]. Additionally, over 30,000 MW of generation were forced off the system with 1,045 individual generating units (e.g., 604 natural gas, 25 coal, 285 wind and 22 solar) experiencing outages.

Figure 1 shows the capacity in ERCOT that could respond to the load decreasing throughout Uri and dropping below the energy emergency alert (EEA) level 3 until significant load shed took place.

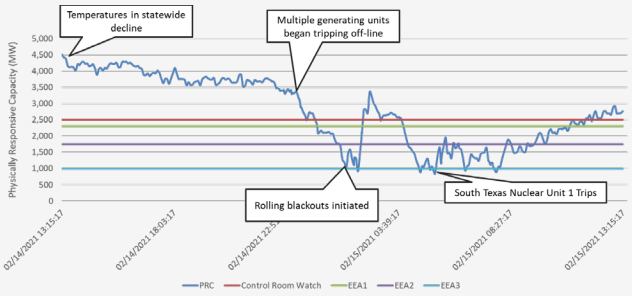


Figure. 1 ERCOT physically responsive capacity [3]

A significant cause of the loss of capacity came from the loss of natural gas production in Texas due to freezing at the wellheads (Figure 2). By February 16, 2021, over 8 billion cubic feet (bcf) of natural gas were shut-in across Texas. Moreover, the gas shut-in affected regions far beyond Texas, as the state is a major supplier of natural gas to several entities throughout the United States including New York Independent System Operator (serviced by the Iroquois Pipeline), PJM Interconnection (serviced by Columbia Gas Transmission pipelines, the East Tennessee Natural Gas Pipeline and the Guardian Pipeline), Midcontinent Independent System Operator (serviced by Natural Gas Pipeline Company of America pipelines) and Western Electricity Coordinating Council (serviced by El Paso Natural Gas, Transwestern Pipeline Company and WBI Energy pipelines and the Rockies Express Pipeline) [4].

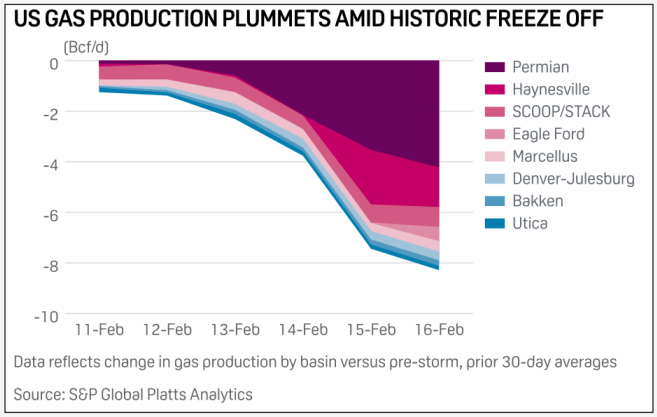


Figure 2. Gas production freeze offs [5]

The impact of Uri led to significant proposed changes throughout ERCOT and the Texas Railroad Commission (TRC), the entity that oversees and regulates natural gas and oil operations in Texas. These proposed changes were in the form of House and Senate bills within the state legislature, recommendations from the Federal Energy Regulatory Commission (FERC) and North American Electric Reliability Corporation (NERC) and projects per the Public Utility Commission of Texas (PUCT).

The legislative changes within the state House and Senate include three separate bills

- Texas House Bill 1510 opens up securitization for utilities, allowing them to recoup costs for winter modifications and creating the Texas Electric Utility System Restoration Corporation. This bill allows funding of utilities to prepare for future weather and provides a way for the funds to be proactive. It also allows improved restoration of electricity back to the grid during inclement weather.
- Senate Bill (SB) 2 states that ERCOT's board will decrease from 16 to 11 members. It is important to note that 9 of the 11 board members will have voting powers.
- SB 3 allows ERCOT and TRC to identify critical components of the natural gas/energy system and require they be protected from the cold. This protection only applies to equipment directly linked to power plants and does not include new facilities, transmission lines and pipes connected to customers. If existing facilities do not comply with weatherization, a penalty of up to $1 million will be assessed per offense. ERCOT will establish further penalty guidelines. SB 3 also implements education and communication systems for extreme weather and sends a grid reliability report to the state legislature every even year. Lastly, a $6.5 million fund will cover the cost ratepayers incurred during winter 2021.

// PERSPECTIVES (cont'd)

On November 16, 2021, FERC and NERC issued their final report on Uri and recommendations [4]. The first few recommendations suggest that generator owners identify and winterize critical components. This winterization must consider precipitation and wind, and not base it on ambient air temperatures. Recommendations that follow ask generator owners to revise and analyze the cold weather preparedness of each unit annually. The inspections of these winterizations should take place pre-, mid-, and post-winter. If these generators experience a weather-related outage, they must review their cold-weather plan and modify it to correct the problem. The owners of the units will be compensated through markets or PUCT for complying with the recommendations of winterization and other weather-related outage preparedness. The generator owners, operators and balancing authorities must also define their respective roles in determining the amount of energy that can reliably be distributed in extreme weather events.

The subsequent recommendations are directed toward grid operations and planning for extreme weather. To improve grid operations, all critical natural gas infrastructure is prohibited from being used as a demand response. Transmission owners must also have individual circuits used for manual, underfrequency and critical load shed. When planning for inclement weather, it is vital to abide by the bills and recommendations discussed previously. Additionally, transmission owners can review and improve load shedding plans. Balancing authorities should amend rules to reduce time to report any outages. Provisions should be enacted to make corrections to address natural gas supply shortfalls.

Although the actions spelled out in these bills and recommendations are needed to prevent another disastrous outage, there must be a vehicle by which these changes can be enabled. This is where PUCT comes in with their proposed projects [6, 7, 8, 9, 10, 11, 12, 13], each of which sets a framework for the implementation of rules which ensure the winterization of key electric systems and improved preparedness for all other infrastructure and markets. These advancements would prevent an outcome similar to that of Winter Storm Uri.

Unfortunately, many of the proposed bills, FERC and NERC recommendations and PUCT projects have yet to be implemented. Moreover, the TRC has moved more slowly. A proposal published in September 2021 lays out a timeline that would identify, map and impose weatherization mandates by early 2023 for gas producers that supply power plants. However, the proposed rule allows gas companies to opt out of that category and avoid having to weatherize their equipment. With natural gas availability making up one of the most significant issues during Uri, the opt-out and lack of expedience of the TRC in addressing the weatherization issues leaves the residents of Texas vulnerable to future issues if a major freeze were to again hit the state. – Contributed by **Robert Wallace***, **Nicholas Messina*** and **Victoria Toetz*** in support of SSAE's Energy Markets Analysis Team

References

[1] NPR, "Texas officials put the final death toll from last year's winter storm at 246," January 3, 2022.

[2] Texas Comptroller, "Winter Storm Uri 2021, The Economic Impact of the Storm," October 2021.

[3] ERCOT, "Historical Real-Time ORDC and Reliability Deployment Price Adders and Reserves – February 2020," 2021.

[4] FERC, "FERC - NERC - Regional Entity Staff Report: The February 2021 Cold Weather Outages in Texas and the South Central United States," November 16, 2021.

[5] S&P Global, "Midcon, Texas gas prices hit records; polar weather throws US market off kilter," 2021.

[6] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51825," 2022.

[7] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51830," 2022.

[8] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51839," 2022.

[9] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51840," 2022.

[10] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51841," 2022.

[11] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51871," 2022.

[12] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51888," 2022.

[13] Public Utility Commission of Texas, "Interchange Filing Search, Filings for 51889," 2022.

// UPCOMING

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

CERAWEEK 2022
Attendee: **Luciane Cunha**
Houston, TX, March 7–11, 2022

// RECENT PUBLICATIONS

Models/Tools/Databases

K. Buchheit*, **A. Noring***, **A. Iyengar*** and **G. Hackett**, "Solid Oxide Cell Manufacturing Cost Tool," National Energy Technology Laboratory, Pittsburgh, PA, January 2022.

National Energy Technology Laboratory, "NETL CO2U LCA Documentation Spreadsheet," National Energy Technology Laboratory, Pittsburgh, PA, February 23, 2022.

National Energy Technology Laboratory, "NETL CO2U LCA Guidance Toolkit – Version 2.0," National Energy Technology Laboratory, Pittsburgh, PA, February 23, 2022.

National Energy Technology Laboratory, "NETL CO2U openLCA LCI Database Version 2," National Energy Technology Laboratory, Pittsburgh, PA, February 23, 2022.

Reports/Supporting Documentation

K. Buchheit*, **A. Noring*** and **A. Iyengar***, "Solid Oxide Cell and Stack Manufacturing Cost Tool," National Energy Technology Laboratory, DOE/NETL-2022/3230, Pittsburgh, PA, January 14, 2022.

T. Skone, **M. Mutchek***, **M. Krynock**, **S. Moni***, **S. Rai***, **J. Chou***, **D. Carlson***, **M. Jamieson**, **E. Dale**, G. Cooney and A. Kumar, "Carbon Dioxide Utilization Life Cycle Analysis Guidance for the U.S. DOE Office of Fossil Energy and Carbon Management, Version 2.0," National Energy Technology Laboratory, DOE/NETL-2022/3774, Pittsburgh, PA, February 23, 2022.

M. Jamieson, **M. Krynock**, **S. Moni***, **M. Mutchek*** and **T. Skone**, "NETL 45Q Addendum to the CO2U LCA Guidance Toolkit," National Energy Technology Laboratory, DOE/NETL-2021/2852, Pittsburgh, PA, February 23, 2022.

National Energy Technology Laboratory, "NETL 45Q LCA Report Template," National Energy Technology Laboratory, Pittsburgh, PA, February 23, 2022.

Conference Proceedings and Events

M. Drouven, "An Optimization Framework for Produced Water Management and Beneficial Reuse," presentation at the 2021 Produced Water Society Seminar, Virtual, September 8, 2021.

M. Drouven, "An Optimization Framework for Produced Water Management and Beneficial Reuse," presentation at the National Alliance for Water Innovation (NAWI) Modeling & Simulation Seminar Series, Virtual, September 15, 2021.

D. Miller, "Optimizing Innovative Process and Energy Systems of the Future," presentation as part of the Texas A&M Energy Institute 2021–2022 Lecture Series, Hybrid (Virtual and College Station, TX), January 26, 2022.

S. Zitney, " Virtual Digital Twin for Real-Time Integrated Power Plant Control Room and Field Operations Research, Training, and Education," presentation at DOE SMART Initiative webinar, January 27, 2022.

* NETL Support Contractor

// REFERENCE SECTION

Models / Tools / Databases

FE/NETL CO_2 Transport Cost Model

FE/NETL CO_2 Storage Cost Model

FE/NETL CO_2 Prophet Model

FE/NETL Onshore CO_2 EOR Cost Model

Life Cycle Analysis Models

NETL LCA CO2U toolkit

IDAES Power Generation Model Library

Pulverized Coal Carbon Capture Retrofit Database (CCRD)

Natural Gas Combined Cycle CCRD

Industrial Sources CCRD

Key Reports

Baseline Studies for Fossil Energy Plants

Quality Guidelines for Energy System Studies

Life Cycle Analysis

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Life Cycle Analysis webpage

CCSI² webpage

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