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

SSAE Develops Prototype of Flexibility Analysis Tool for IES Design

NETL and collaborators within the Institute for the Design of Advanced Energy Systems (IDAES) prototyped a new optimization tool for analyzing the flexibility of integrated energy system (IES) designs. The tool measures the size of the uncertain parameter space over which feasible steady-state operation of an IES design can be attained by proper adjustment of process control variables. The tool was demonstrated on an interconnected network of four IDAES heat exchanger models. The inlet flows and temperatures of two process inlet streams were specified as uncertain parameters. Control variables included the inlet flow of a cold process stream and a cooling duty. The resulting mixed integer nonlinear programming problem was solved in IDAES using both vertex enumeration and sampling algorithms. Flexibility test results showed that the network design was infeasible and identified the critical point representing maximum constraint violation. Work is underway to apply the tool to a solvent-based carbon capture process and integrated power and hydrogen co-production system. The prototype and demonstration results were highlighted at the virtual IDAES Stakeholder Workshop in October 2021.

SSAE's EMAT Participates in Energy Storage Grand Challenge

Members of SSAE's Energy Market Analysis Team participated in the Community of Practice presentation series, part of the Policy & Valuation (P&V) Group of the Energy Storage Grand Challenge (ESGC), in November 2021. A presentation describing the value of energy storage (ES) for fossil energy (FE) from two perspectives, 1) a market-based valuation from the perspective of the ES developer and power generation sector and 2) a system-based valuation, was given by **Ivonne Pena-Cabra***. The presentation also provided a detailed description of the relevant market, regulatory and policy characteristics that can provide economic signals for the integration of ES-FE concepts in the Midcontinent Independent System Operator and Electric Reliability Council of Texas.

Despite the holiday, there was great attendance. ESGC P&V leadership is looking forward to link the analysis presented to a larger ESGC valuation theme, and to continue partnering with NETL on ESGC topics beyond those of the presentation. Some potential avenues for continued partnership between NETL and ESGC include hybridization, optimization for market bidding, assessment management aspects of integration and siting and sizing.

New Version of FOQUS Available as Part of CCSI Toolset

Version 3.11.0 of the Framework for Optimization and Quantification of Uncertainty and Surrogates (FOQUS) software, part of the Carbon Capture Simulation Initiative (CCSI) Toolset, was released by the Carbon Capture Simulation for Industry Impact (CCSI^2) team. FOQUS is a platform that can integrate numerous models in different platforms (e.g., Aspen, Excel, Python, MATLAB, etc.) and seamlessly conduct optimization and uncertainty quantification on the integrated model. The new version improved documentation for the Sequential Design of Experiments module, is compatible with Python 3.8 and fixed compatibility issues. The new release will enhance capabilities in guiding optimal experimental design (maximize value of data collected) and coupling data collection with improvements in multi-scale modeling. The FOQUS release improves NETL's capabilities in advancing carbon capture technologies through technology readiness levels via improvements in process design, uncertainty quantification, optimization and enhanced lab, bench and pilot data collection.

SSAE Advances Estimating Costs of Integrated SOFC Systems

SSAE is evaluating the economic feasibility of different IES leveraging NETL's capital cost scaling and IDAES capital cost methodology which consists of using SSAE's existing engineering, procurement, and construction or vendor quotes for estimating capital costs of major equipment and/or main components in energy systems.

The IDAES capital costing methodology was recently updated to support solid oxide fuel cell (SOFC) estimation. Accomplishments included 1) adding capital cost scaling for SOFC technologies, air separation units and carbon purification units, 2) revising units of measurements to simplify evaluating different technologies under market analysis, 3) extending the library to support fixed and variable operation and maintenance costs, 4) providing correlations to calculate total owner cost, total as spent cost and annualized cost, and 5) developing the workflow to evaluate surrogate models for fixed and variable costs of the technologies. Future work will focus on developing a workbook that includes all the surrogate models for different technologies under this effort.

A Jupyter Notebook (a tool for interactive computing across dozens of programming languages) was prepared for interfacing each technology with a market analysis problem. Given the importance of decarbonizing the U.S. energy system, it is assumed that CCS is needed for all cases, so each process concept will be analyzed under different market scenarios to rank the optimized process options. Additionally, this work has been used to test the new IDAES surrogate API demonstrating the end-to-end workflow for reading data, training surrogate models and importing surrogate models for optimization.

SSAE Contributes to Congressional Report on REE/CM Program Success

NETL and the Office of Fossil Energy and Carbon Management (FECM), in compliance with a statutory requirement and with leading contributions from SSAE, are submitting a Report to Congress on the achievements of FECM's Rare Earth Elements and Critical Minerals (REE/CM) program since its inception in 2015. SSAE's **Tom Tarka** is lead author in summarizing the accomplishments of NETL's Research & Innovation Center

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// HIGHLIGHTS cont'd

(RIC) and the successes of the extramural program in 1) characterizing the resource and its extent, 2) validating and scaling up processes to produce high-purity REEs/CMs from unconventional resources including coal and materials from legacy mining and coal utilization operations (e.g., coal refuse, coal ash), and 3) developing techno-economic analysis (TEA) frameworks and performing TEAs to inform process development and compress the time required to create a new domestic industry to produces these materials.

Infrastructure Bill Presents Opportunities and Challenges for SSAE

In November 2021, Congress passed, and the President subsequently signed, a nominally bipartisan infrastructure bill, called the Infrastructure Investment and Jobs Act. According to the White House statement on the bill's passage, this deal will:

> *"…rebuild America's roads, bridges and rails, expand access to clean drinking water, ensure every American has access to high-speed internet, tackle the climate crisis, advance environmental justice, and invest in communities that have too often been left behind. The legislation will help ease inflationary pressures and strengthen supply chains by making long overdue improvements for our nation's ports, airports, rail, and roads. It will drive the creation of good-paying union jobs and grow the economy sustainably and equitably so that everyone gets ahead for decades to come."*[1]

The law provides authorizations for $1.2 trillion worth of federal spending on infrastructure and other investments, including $550 billion of new spending, over the next five years. It is important to note that Congress will still need to appropriate money to fund this authorized spending in each year's budget.

Much of the spending, indeed, well over 50% of the new authorizations, are focused on traditional concrete and steel infrastructure such as roads, bridges, rail, airports and waterways. Even though this legislation is not explicitly an energy or climate bill, it describes new priorities and initiatives which modify previous energy bills and has many indirect connections to energy systems and decarbonization strategies via investments in electrical grid infrastructure, resiliency and environmental remediation efforts and electric vehicles.

Even with the understanding that energy and climate are not the focus, the scale of this spending is such that there are still enormous opportunities for NETL and SSAE. The broad analysis capabilities and expertise therein are critical to effective allocation of this funding. It is likely that without any significant effort, increased scope and associated funding will end up on our collective plate in traditional areas such as carbon capture, transport, storage and utilization.

Perhaps the more exciting opportunities lie in identifying and actively positioning NETL and SSAE to lead or have significant collaborations in emerging areas described and funded within the bill such as hydrogen or critical materials supply chains. Aligning these opportunities with the existing capabilities and proposed strategic capability investments is an ongoing priority for SSAE and RIC leadership.

This level of funding also presents challenges for growth for an organization whose strength is its people. Already SSAE is seeing increased demand for its people and services as momentum continues to build for the energy and climate transition worldwide and the associated need for sound analytical underpinnings. Finding the right people to join the team to meet the new demands of the infrastructure bill is an effort that will require exercising the networks of the entire existing staff, but that challenge can be met with the opportunity as a sales pitch. It is an exciting time to join an energy analysis organization.

Reference

[1] The White House, "Fact Sheet: The Bipartisan Infrastructure Deal," https://www.whitehouse.gov/briefing-room/statements-releases/2021/11/06/fact-sheet-the-bipartisan-infrastructure-deal/, November 6, 2021.

// NOTICES

SSAE Water Treatment Modeling Tool Released and Rebranded

In September 2021, SSAE, in collaboration with Lawrence Berkeley National Laboratory, National Renewable Energy Laboratory and Oak Ridge National Laboratory, publicly released ProteusLib, a water treatment model library compatible with NETL's IDAES Platform. SSAE researcher **Tim Bartholomew** led the development of the tool as part of the National Alliance for Water Innovation (NAWI). The model library supports detailed analyses of full water treatment trains and spans chemical and physical pretreatment, reverse osmosis (RO) desalination and chemical post-treatment process. Specific use case demonstrations have included techno-economic assessments of low salt rejection RO and high-pressure RO and the creation of a digital twin for an operating seawater desalination plant. As of October 1, ProteusLib was rebranded as WaterTAP. Learn more.

SSAE Part of Awarded COGENT Proposal

The Process Systems Engineering Research Team/CCSI^2 team will be partnering with the University of Sheffield's Translational Energy Research Centre (TERC), SSE Thermal, AECOM Ltd, National Carbon Capture Center (NCCC) and Technology Centre Mongstad DA (TCM) on the awarded "Capture Operation for Generating Electricity while Negating Transients" (COGENT) proposal. Each entity will be funded by their government; in the case of CCSI^2, by the U.S. Department of Energy (DOE). This project will provide insight on operation of capture plants under highly variable market conditions, drawing on both modeling expertise and pilot-scale data validation. Knowledge gained will greatly improve NETL's knowledge and capabilities in flexible capture systems.

Dynamic modeling of monoethanolamine-based CCS will be performed by CCSI^2 and validated with small- (TERC) through large-pilot (NCCC, TCM) data generation. COGENT will support acceleration of the deployment of highly flexible CCS processes which will sustain high rates of CO_2 capture (95%+) through all operational modes and transients of natural gas combined cycle power generation.

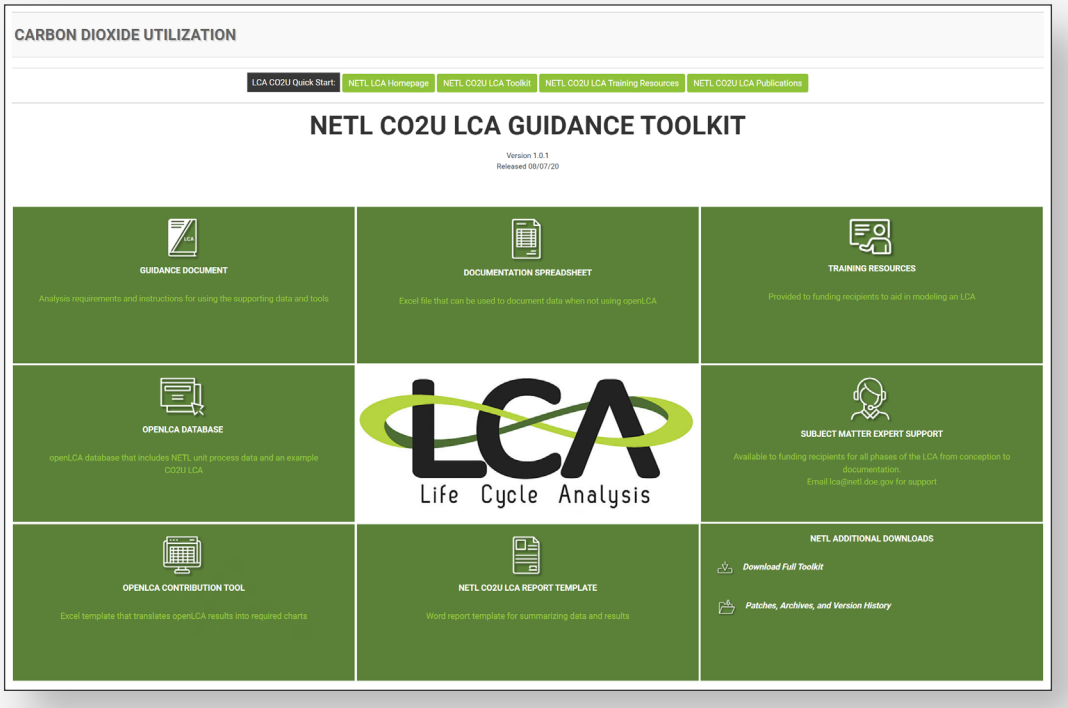
NETL to Release New Version of CO2U LCA Guidance Toolkit

Carbon utilization can reduce greenhouse gas 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 NETL CO2U LCA Guidance Toolkit is intended to help DOE Carbon Utilization Program project principal investigators meet life cycle analysis (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. 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.

Public release is awaiting regulatory approval.

Screenshot of publicly available NETL CO2U LCA Guidance Toolkit



// SSAE CORE CAPABILITIES

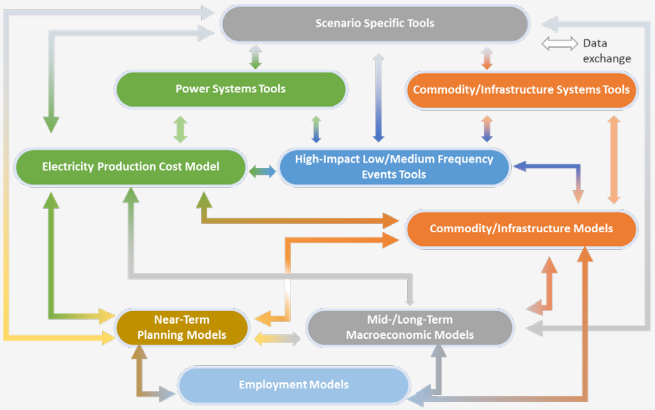
Energy Market and Infrastructure Analysis at NETL

Energy Markets and R&D Benefits Analysis

NETL relies on SSAE's Energy Markets Analysis Team (EMAT) to provide economic, market and regulatory analysis to support RIC in guiding, evaluating and justifying research, development and demonstration (RD&D) programs and in performing other activities ancillary to NETL's core RD&D mission. EMAT has expertise in evaluating the potential role of advanced technologies being developed by NETL research and development (R&D) for competitiveness in the future U.S. energy landscape under varying factors including market forces, macroeconomic trends and government regulations. Scenario analyses use platforms, such as the Market Allocation (MARKAL) or other macroeconomic models and various pipeline and electric grid infrastructure models, with regional, national or global focus (an example of MARKAL results is shown in Figure 1). Characterization of the upstream resources (e.g., coal, natural gas and liquids including water) critical to energy production also form a vital part of these analyses.

Furthermore, EMAT conducts studies to evaluate potential benefits of NETL programs to ensure that the R&D investments not only contribute to the achievement of DOE missions but do so with a significantly positive economic impact regionally as well as nationally. In addition to custom model development, EMAT capabilities include utilization of input-output models and in-house-developed econometric models to assess regional and national economic impacts, including those on employment and gross domestic product. EMAT takes many of the tools that are already utilized in industry and brings them together into a single continuum as opposed to the silos in which they often reside, as shown in Figure 2.

Figure 2. Industry tools brought together by EMAT into single continuum



Economic Dispatch and Energy Infrastructure Modeling

The goal of R&D is to improve existing plant performance and develop new power plants to meet changing market needs. Understanding how technology translates to market penetration depends on the plant's ability to acquire fuel and dispatch into its regional electricity market. Using economic dispatch, capacity expansion and infrastructure forecasting models allows EMAT to provide feedback to researchers on cost targets. Additionally, economic dispatch modeling is used to predict grid reliability issues as more baseload energy is retired and replaced by renewables and natural gas, which have some regional infrastructure constraints. Answers to these questions result in a more resilient energy infrastructure network as the system continues to transition.

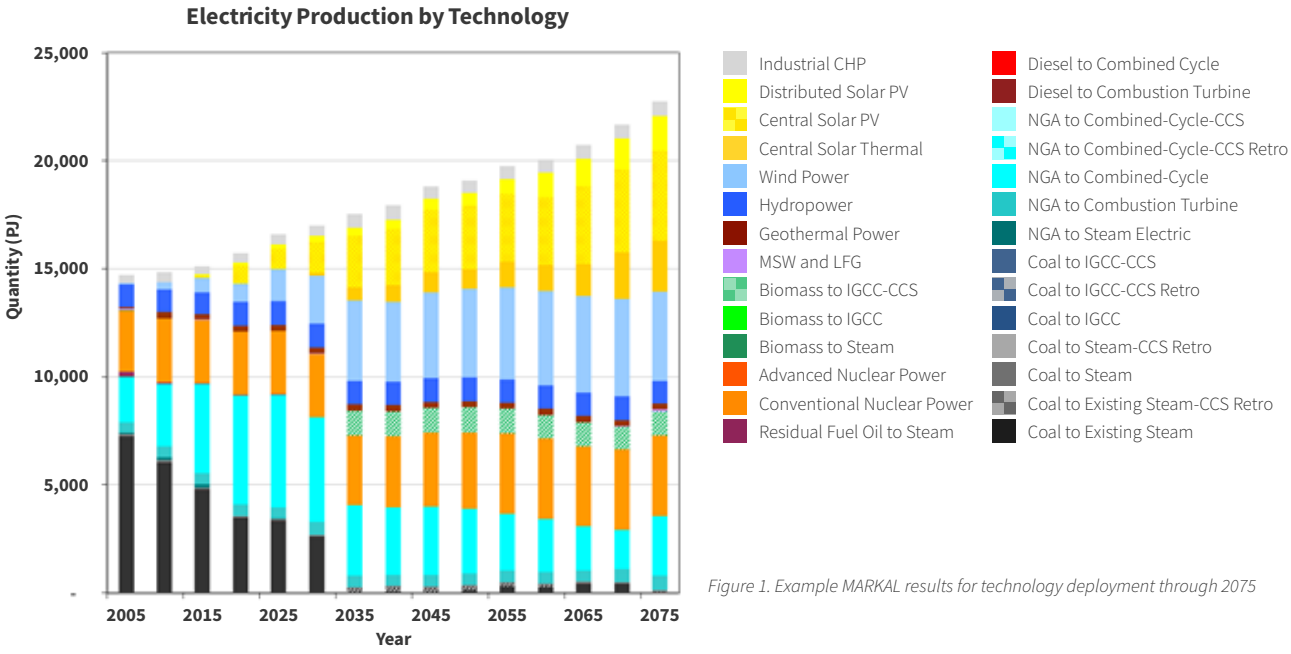


Figure 1. Example MARKAL results for technology deployment through 2075

// SSAE CORE CAPABILITIES (cont'd)

EMAT provides analytical expertise for energy infrastructure analysis across the energy value chain including the gathering, transporting, storing and processing of primary energy products, their conversion into products and associated byproducts and the ultimate consumption/use of products and byproducts. EMAT's analysis includes but is not limited to the national electric power grid, transportation of energy commodities (e.g., pipeline, rail, barge, etc.) and end uses such as heating and cooling, industrial processes and other purposes. For example, in a future scenario that relies heavily on natural gas power generation without the necessary investment in pipeline infrastructure, reliability and resiliency issues would likely occur. Using its suite of models and tools, EMAT is able to project natural gas demand for power generation (Figure 3) given a set of assumptions in a given region. Based on those projections, EMAT can analyze the current infrastructure (in this case, natural gas pipelines) to determine if additional build-out (or investment) is necessary to meet the projected demand. In this scenario, the additional pipeline infrastructure requirements are represented by the blue bars in Figure 4. – Contributed by **Justin Adder**, SSAE's Energy Markets Analysis Team

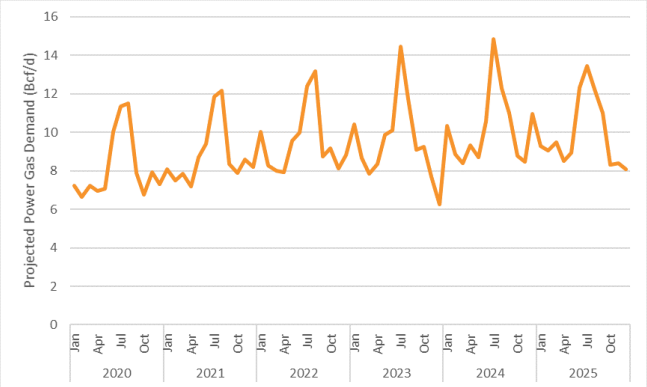


Figure 3. Natural gas demand for future scenario example

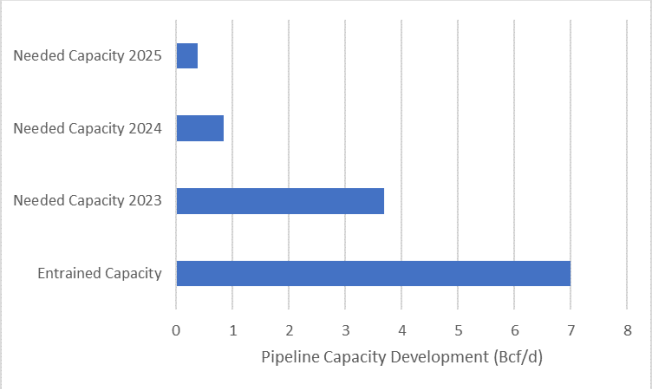


Figure 4. Pipeline infrastructure requirements for future scenario example

// UPCOMING

SSAE Federal staff and NETL Support Contractor personnel will attend or present at the following meetings and conference in January 2022:

- American Economic Association (AEA)/Allied Social Science Associations (ASSA) 2022 Annual Meeting
  Peter Balash (participant)
  Virtual, January 7–9, 2022
- Texas A&M Energy Institute Lecture Series
  David Miller (presenter)
  College Station, TX, January 26, 2022
- POWERGEN International 2022 Conference
  Sydney Hughes (participant)*
  Dallas, TX, January 26–28, 2022

// CONFERENCES AND EVENTS

- AEA/ASSA 2022 Annual Meeting
  Virtual, January 7–9, 2022
- Texas A&M Energy Institute Lecture Series
  College Station, TX, January 26, 2022
- POWERGEN International 2022 Conference
  Dallas, TX, January 26–28, 2022

// RECENT PUBLICATIONS

Conference Proceedings and Events

E. Hedrick, K. Reynolds, V. Dwivedy, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Modeling and Control of an Industrial Selective Catalytic Reduction Unit with Model Predictive Control and Reinforcement Learning," presentation at the 45th International Conference on Clean Energy – The Clearwater Clean Energy Conference, Virtual, July 29, 2021.

L. Henthorne, J. Ciferno, **M. Drouven**, K. Work and D. Agarwal, "Project PARETO: An Optimization Framework for Produced Water Management and Beneficial Reuse," presentation at PARETO Initial Stakeholder Board Meeting, Virtual, September 22, 2021.

M. Krynock*, **B. Young*** and **T. Skone**, "NETL CO2U LCA Guidance Toolkit Introduction," presentation to the Fossil Energy and Carbon Management Carbon Use Welcome Session for algae-based projects, Virtual, October 25, 2021.

G. Hackett, "Solid-State Electrochemical Cell, R&D Progress at NETL," *Proceedings of the 22nd Annual SOFC Project Review Meeting*, Virtual, November 17, 2021.

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// 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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