Carbon Capture Simulation for Industry Impact ($CCSI^2$)

primary project goal

The primary goal of the Carbon Capture Simulation for Industry Impact ($CCSI^2$) project is to utilize the computational tools and models developed under the Carbon Capture Simulation Initiative (CCSI) in partnership with industry to accelerate and de-risk the scale-up of new and innovative carbon capture technology. The $CCSI^2$ operates in conjunction with and in support of the U.S. Department of Energy's (DOE) Office of Fossil Energy and Carbon Management (FECM) to focus on advancing promising technologies.

In 2010, DOE initiated CCSI to help reduce the amount of time that it historically takes to develop and scale-up new technologies in the energy sector, which traditionally takes up to 15 years to move from the laboratory to pre-deployment, and another 20 to 30 years for mature, industrial-scale deployment. Advanced modeling and simulation is developed and applied to enable more rapid and lower-cost capture technology development at reduced risk during the commercialization process.

technical goals

The team assists the Carbon Capture Program and technology developers by providing:

- Detailed understanding of capture materials through system performance under parametric uncertainty.
- Designs for high performance and intensified unit operations.
- Synthesis of processes optimized for novel materials.
- More informed design, operating, and control decisions.
- Modeling, optimization, and test campaign support for small and large pilots.
- Optimized processes under uncertainty.
- Intelligent design of experiments (DoE) at all Technology Readiness Levels (TRLs) for model refinement, system optimization, and acceleration of deployment.
- Machine learning (ML) frameworks to reduce computational time.
- Support for the Framework for Optimization and Quantification of Uncertainty and Surrogates (FOQUS), which will centralize and integrate computational capabilities critical to the Carbon Capture Program and $CCSI^2$ mission.

technical content

In support of the Carbon Capture Program, $CCSI^2$ maintains the CCSI Toolset, released to the public as open-source software, and continues to prepare tools, document capabilities and instructions for use, manage a public repository, and implement a release management system for subsequent versions of the tools.

$CCSI^2$ is led by the National Energy Technology Laboratory (NETL) and leverages the DOE national laboratories' core strengths in modeling and simulation. In full pursuit of the $CCSI^2$ vision, this project integrates the modeling and simulation capabilities at NETL and complements them with essential, world-class expertise

project focus:
Advancing Carbon Capture Technology Scale-Up

participant:
National Energy Technology Laboratory–Research and Innovation Center

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predecessor project:
2020 $CCSI^2$ FWP

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at Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Pacific Northwest National Laboratory (PNNL), and Oak Ridge National Laboratory (ORNL) in its core national laboratory consortium.

Carbon capture is critical to significantly reducing domestic and global carbon dioxide (CO_2) emissions. However, the energy and capital cost associated with carbon capture systems is prohibitive for deployment. Today's cost to capture CO_2 using state-of-the-art carbon capture technologies must be reduced to competitive levels more rapidly and at lower risk. FECM goals are for technologies under development to be ready for commercial deployment by 2030 and must be on a pathway to capture at least 95% of generated CO_2 and achieve 20% reduction in captured cost for natural gas combined cycle (NGCC) power plants relative to the baseline case without carbon capture and storage (CCS; excluding transportation and storage costs). Prior requirements for 90% CO_2 capture have been increased, which introduces the challenge of increasing CO_2 capture while mitigating cost increases. Balancing cost management with a high level of CO_2 capture meaningful enough to contribute to climate change mitigation is critical in this new approach, yet the balance introduces a great deal of additional complexity. $CCSI^2$, with proven cost-performance optimization frameworks, is ideally positioned to apply the CCSI Toolset to provide well-informed perspective on the most impactful areas of research to achieve these more aggressive decarbonization goals.

The $CCSI^2$ team provides fundamental analysis, modeling, and optimization of carbon capture technology by working closely with industry partners. The $CCSI^2$ team efficiently identifies data collection needs, computationally and experimentally characterizes carbon capture materials, designs and optimizes prototype devices and processes, and fully propagates uncertainty in model predictions for a complete perspective on results accuracy.

For Execution Year 2022 (EY22), the work is organized under several tasks, including NGCC Pilot Support, General Capture R&D Program Support, CCSI Toolset Community Support, and Support for Industrial Capture Applications. The task for General Capture Program support focuses on increasing the impact of research and development (R&D) by generating and applying computational frameworks to support carbon capture technology research. The subtasks include Computational and Experimental Support for CO_2 Absorber Process Intensification, Monoethanolamine (MEA) Modeling and Cost Analysis of High Capture Rates, and Robust Optimization of Solvent-based System Designs.

The CCSI Toolset Community Support task manages the open-source CCSI Toolset and facilitates active development, deployment, and maintenance of the CCSI Toolset software, with updated features, capabilities, and documentation, by and in support of the research efforts within other subtasks of $CCSI^2$. This subtask includes the development of Sequential Design of Experiments (SDoE) to optimize experimental data generation, and development of Machine Learning approaches to increase the efficiency of the computational fluid dynamics models that support process intensification. This subtask also includes the education of contributing developers from these subtasks on mature software development practices and tools, as well as active support and outreach to new users and stakeholders.

The Pilot Support task supports Carbon Capture Program projects scheduled for pilot testing of carbon capture technologies at Technology Centre Mongstad (TCM). Support includes the development of materials, device, and process models with sufficient uncertainty quantification to support the DoE required to maximize knowledge gained from the TCM test campaigns. The aim is to leverage and improve modeling during each campaign to reduce the time and cost while maximizing productivity of each campaign. Four technology developers will be piloting solvent-, membrane-, and sorbent-based capture technologies and all will require DoE support. Each technology developer is also interested in optimizing their system's operation and potential configuration to reduce thermodynamic penalties, reduce cost, and minimize environmental impact (e.g., solvent emissions).

The $CCSI^2$ EY22 tasks have seven thrusts:

1. Provide direct support to the small natural gas pilot projects recently awarded by the Carbon Capture Program. This work ensures advanced materials development efforts are integrated with advanced systems design, analysis, and optimization, as well as supports SDoE to maximize the value of the test campaign. Additionally, the desired outcome is to enhance computational capabilities for generalized natural gas solvent and sorbent frameworks for multi-scale, integrated materials, device, and process optimization.
2. Develop a formalized SDoE methodology that will strive for data generation at all TRLs that is optimized for a variety of objectives (i.e., model refinement, process optimization, etc.). The desired outcomes are to continue adding relevant capability for computational SDoE for steady state and dynamic processes into FOQUS. This includes non-uniform space filling and input response space filling experimental designs, which more effectively leverage and inform equation-based modeling efforts than more conventional uniform space filling approaches. SDoE focuses on maximizing learning while reducing the time and cost of generating useful experimental results. SDoE can also be used to increase the efficiency of computationally intense, simulation-based experimentation; develop constrained

experimental designs to consider operational and/or safety restrictions; and develop experimental designs to focus on exploration of model output directly relevant to programmatic goals.

3. Inform R&D efforts in projects supported by the Carbon Capture Program through fundamental modeling, analysis, and optimization. The desired outcomes are the continued development of a modeling framework that supports superstructure-based advanced flash stripper process synthesis framework for generic solvents, accurate wetted area calculational framework for estimating generic packing and generic solvents to inform device performance, and transfer lessons learned from coal-based modeling to natural gas-based applications.
4. Support the open-source release of the CCSI Toolset. The desired outcome is to upgrade the open-source Toolset release to communicate with more modeling platforms required for the direct support of the Carbon Capture Program, including interfacing with a new ML tool under development that will automate the development of surrogate computational fluid dynamics (CFD) models.
5. Continue to support the Carbon Capture Program projects funded to pilot their CCS technology at TCM. The desired outcomes are to complete modeling of Research Triangle Institute's (RTI) non-aqueous solvent (NAS) system performance and aerosol emissions, which will support the SDoE for the TCM pilot tests, and continue Membrane Technology and Research Inc. (MTR) membrane modeling and TDA Research Inc. (TDA) sorbent modeling, which will support their own SDoE.
6. Continue device-scale intensification and optimization. The desired outcomes are to continue computationally developing intensified device designs that will consolidate process operations, reducing equipment requirements and improving performance. $CCSI^2$ will provide computational designs that can be realized with cutting-edge 3D-printing technology and that will provide performance improvement beyond that of conventional equipment; develop equipment models that fully characterize solvent-packing interactions including hydrodynamics, heat/mass transfer, and solvent chemistry; reduce the computational complexity by integrating with ML approaches to increase the speed of convergence while sustaining high predictive accuracy; and work with the 3D-printing community to use intensified CO_2 capture absorber modeling to inform advanced manufacturing processes.
7. Support industrial CCS. The desired outcome is to provide an understanding of how CCS could be integrated into a cement plant such that tradeoffs between the techno-economic performance of the CO_2 capture system and its effects on the base cement plant and product quality are optimally balanced.

technology advantages

The $CCSI^2$ team engages carbon capture technology developers for direct and widespread support of priority interests of the Carbon Capture Program with the aim to fully understand and exploit the unique behavior of recently developed transformational carbon capture materials and equipment. $CCSI^2$ continues developing a technical understanding of CO2 system operation in ways that will serve to guide R&D required for an electrical grid evolving to incorporate more intermittent renewables. $CCSI^2$ is constantly developing a more comprehensive understanding of CO_2 capture technology for applications including natural gas and industrial sources, at increasing and deeper levels of decarbonization. $CCSI^2$ is also positioned to address issues related to direct air capture of CO_2 to effectively address the more difficult to decarbonize sectors like transportation.

The open-source CCSI Toolset (1) enables promising concepts to be more quickly identified through rapid computational screening of materials, equipment, and processes; (2) reduces the time to understand, design, and improve new, intensified devices by developing detailed device-scale models; (3) fundamentally characterizes steady state process operation and dynamic process operation for extended understanding of process flexibility and control; (4) optimizes process design with a suite of state-of-the-art algorithms that target the best overall operating conditions and process configurations; (5) provides a comprehensive computational framework for systematic experimental design optimal to the objectives defined by the testing protocol; and (6) provides quantitative predictions of material, device, and process performance during scale-up based on rigorously validated simulations that take into account model and parameter uncertainty.

R&D challenges

- Identification and rigorous quantification of scale-up uncertainty and model enhancement to reduce such uncertainties.
- Technology-specific challenges in development of various transformational carbon capture materials and equipment.

status

CCSI[2] released the FOQUS version 3.13.1; support for the software continues to fix bugs and add capabilities directly supporting the analysis needs of the Carbon Capture Program. CCSI[2] is continuing collaboration with three technology developers to support pilot tests of their carbon capture technologies at TCM over the next three years. Collaboration with RTI continues under the Non-Disclosure Agreement (NDA) with NETL, which permits sharing of models and data. CCSI[2] has initiated Cooperative Research and Development Agreements (CRADAs) with RTI and MTR, which will permit data/model exchange amongst all participating CCSI[2] laboratories to begin collaboration. TDA has collaborated with CCSI[2] by sharing sorbent contactor performance data to support model development for the SDoE of the TCM pilot.

available reports/technical papers/presentations

CCSI[2] Website: *https://www.acceleratecarboncapture.org*.

CCSI Toolset: *https://github.com/CCSI-Toolset/*.

CCSI[2] Publications List: *https://www.acceleratecarboncapture.org/publications*.

"Overview of Carbon Capture Simulation for Industry Impact (CCSI[2]) Project," presented by Michael Matuszewski, 2021 Carbon Management and Oil and Gas Research Project Review Meeting, August 2021. *https://netl.doe.gov/sites/default/files/netl-file/21CMOG_PSC_Matuszweski.pdf*.

"CCSI[2] Brief: Computational Support for the Carbon Capture Program," presented by Benjamin Omell, DOE-NETL's 2020 Integrated Project Review Meeting, October 2020. *https://netl.doe.gov/sites/default/files/netl-file/20VPRCC_Omell.pdf*.

"CCSI[2] Project Overview," presented by Michael Matuszewski, 2018 NETL CO_2 Capture Technology Project Review Meeting, August 2018. *https://netl.doe.gov/sites/default/files/netl-file/M-Matuszewski-CCSI2-Capture-Impact-Simulation.pdf*.

"CCSI[2] and Toolset Support Program Overview and Toolset Introduction," presented by Michael Matuszewski, 2017 NETL CO_2 Capture Technology Project Review Meeting, August 2017. *https://netl.doe.gov/sites/default/files/event-proceedings/2017/co2%20capture/3-Wednesday/M-Matuszewski-CCSI2-Program-Overview.pdf*.