CARBON CAPTURE SIMULATION FOR INDUSTRY IMPACT (CCSI2)

Carbon Capture Simulation for Industry Impact

# BACKGROUND

Near-term and large-scale reduction of carbon dioxide ( $CO_2$ ) emissions from fossilbased electricity sources is critical for mitigating climate change. The Carbon Capture Simulation for Industry Impact ( $CCSI^2$ ) program is focused on developing a fundamental understanding of  $CO_2$  capture technology, which will reduce those emissions.  $CCSI^2$  collaborates with industrial, academic and government partners to disseminate a rigorously quantified understanding of  $CO_2$  capture systems, manage risk and reduce the barriers to technology commercialization. The results are well-informed, accelerated technology transfer processes for timely implementation of technologies that benefit the world.



# NATIONAL ENERGY TECHNOLOGY LABORATORY

### **PROJECT DESCRIPTION**

0.54

(d) H,O Gas Fl

200 time (s)

c) CO, Gas Flow

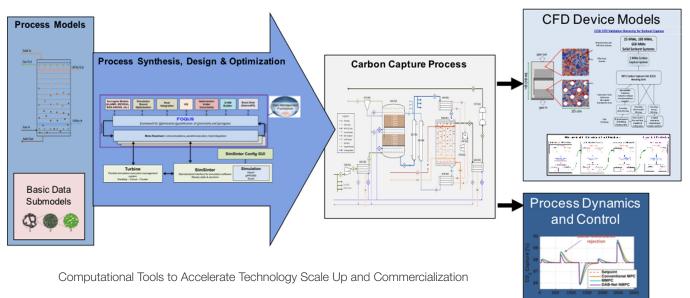
CCSI<sup>2</sup> is led by the National Energy Technology Laboratory (NETL), partnering with Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Pacific Northwest National Laboratory, University of Kentucky, University of Texas at Austin and West Virginia University.

CCSI<sup>2</sup> develops, validates, and applies advanced computational techniques for technology simulation, optimization, uncertainty quantification (UQ), and process control. Computational products are consolidated in the CCSI Toolset software for developing rigorous understanding of CO<sub>2</sub> capture technologies that enable efficient Research and Development (R&D). CCSI<sup>2</sup> develops a detailed multi-scale understanding of the most effective pathways to minimize the cost to capture CO<sub>2</sub>. In FY18 and FY19, CCSI<sup>2</sup> is scoped to directly support ten projects in the Capture Program worth over \$60M in total value while also providing industry-wide benefit by applying a general Design of Experiments (DoE) framework that optimizes large- and small-scale test programs as well as highly accurate benchmark CO<sub>2</sub> solvent system modeling tools.



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## **CARBON CAPTURE SIMULATION FOR INDUSTRY IMPACT (CCSI<sup>2</sup>)**



The primary goal of CCSI<sup>2</sup> is to provide a fundamental and interdependent understanding of CO<sub>2</sub> capture material, device, and system level performance leading to more informed R&D guidance on CO<sub>2</sub> capture technology development and reduced risks during commercialization. To achieve this goal, CCSI<sup>2</sup> will:

- Provide R&D support that reduces risk and increases rate of CO<sub>2</sub> capture technology commercialization
- Generate accurate understanding and guantified uncertainty in CO<sub>2</sub> capture system performance
- Continue to validate, apply and disseminate the CCSI **Computational Toolset**

### **PROJECT BENEFITS**

CCSI<sup>2</sup> is focused on simultaneously accelerating and de-risking research and development of CO<sub>2</sub> capture technologies. Efforts in CCSI<sup>2</sup> reduce the timeline and cost to commercialize technologies capable of cost-effectively achieving deep CO<sub>2</sub> reduction from the fossil fuel power generation industry. Rooted in mathematical optimization frameworks, the computational methods employed by CCSI<sup>2</sup> ensure the best operation, configuration and minimized costs for low carbon fossil fuel generated electricity.

### ACCOMPLISHMENTS/SUCCESSES

CCSI<sup>2</sup> has developed a standard solvent-based CO<sub>2</sub> capture system modeling framework with fundamental, multi-hierarchical characterization that will be used by the international CO<sub>2</sub> capture industry to inform technology testing and development.

Leveraging this fundamental modeling approach, a general framework for optimal steady state design of experiments (DoE) has been applied to pilot scale testing to increase precision of CO<sub>2</sub> capture models to +/-3% in a matter of weeks as opposed to years in conventional approaches. This DoE uses principles of Artificial Intelligence (AI) to generate testing requirements for most efficient and informative experimental data generation. This approach simultaneously improves model uncertainty and maximizes impact of test programs at all scales and technology readiness levels.

CCSI<sup>2</sup> is performing multi-scale optimization of several CO<sub>2</sub> capture systems under development by the Fossil Energy Carbon Capture Program. Projects include: University of Texas at Austin-Advanced Flash CO<sub>2</sub> Regeneration; Lawrence Livermore National Laboratory-1) Micro-Encapsulated CO<sub>2</sub> Sorbent (MECS) and 2) Device Scale Advanced Manufacturing; University of Kentucky-CO<sub>2</sub> Capture Pilot Process Control; Lawrence Berkeley National Laboratory-Metal Organic Frameworks (MOFs); Pacific Northwest National Laboratory-Low-Aqueous Solvents.

Research Partners Leidos Research Support Team (LRST) | Lawrence Berkeley National Laboratory | Lawrence Livermore National Laboratory | Los Alamos National Laboratory Pacific Northwest National Laboratory | University of Kentucky | University of Texas at Austin | West Virginia University

#### Contacts

#### **Benjamin Omell** Technical Project Lead Research Engineer benjamin.omell@netl.doe.gov

#### Michael Matuszewski Associate Technical Director

Carbon Capture Simulation for Industry Impact (CCSP) michael.matuszewski@netl.doe.gov

**David Miller** Technical Director, CCSP Senior Fellow **Process Systems Engineering** david.miller@netl.doe.gov