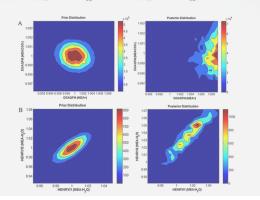


### BACKGROUND



Near-term and large-scale reduction of carbon dioxide  $(CO_2)$  emissions from fossil-based electricity sources is critical for a zero carbon future. The Carbon Capture Simulation for Industry Impact (CCSI<sup>2</sup>) program is focused on developing a fundamental understanding of  $CO_2$  capture technology, which will reduce carbon-based emissions. CCSI<sup>2</sup> 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**

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, Oak Ridge National Laboratory, University of Toledo, University of Pittsburgh, University of Notre Dame, Carnegie Mellon University, University of Texas at Austin and West Virginia University.

 $CCSI^2$  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  $CO_2$  capture technologies that enable efficient Research and Development (R&D).  $CCSI^2$  develops a detailed multi-scale understanding of the most effective pathways to minimize the cost to capture  $CO_2$ . Between FY18 and FY20,  $CCSI^2$  has directly supported ten projects in the Capture Program, with an investment of more than \$80M. Simultaneously,  $CCSI^2$  has provided industry-wide benefit by applying a general Design of Experiments framework that optimizes large- and small-scale test programs, as well as highly accurate benchmark  $CO_2$  solvent system modeling tools.





## 

The primary goal of CCSI<sup>2</sup> is to provide a fundamental and interdependent understanding of  $CO_2$  capture material, device, and system level performance leading to more informed R&D guidance on  $CO_2$  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 quantified uncertainty in CO<sub>2</sub> capture system performance
- Continue to validate, apply and disseminate the CCSI
  Computational Toolset

## **PROJECT BENEFITS**

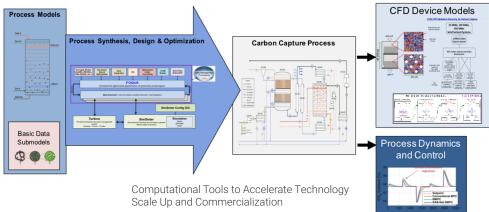
 $\rm CCSI^2$  is focused on simultaneously accelerating and de-risking research and development of  $\rm CO_2$  capture technologies. Efforts in  $\rm CCSI^2$  reduce the timeline and cost to commercialize technologies capable of cost-effectively achieving deep  $\rm CO_2$  reduction from the fossil fuel power generation industry. Rooted in mathematical optimization frameworks, the computational methods employed by  $\rm CCSI^2$  ensure the best operation, configuration and minimized costs for low carbon fossil fuel generated electricity. While initiatives continue to improve fossil fuel processing in the short-term, NETL is working with our partners to achieve a responsible transition in the future to heavier reliance on renewable energy resources.

## **ACCOMPLISHMENTS/SUCCESSES**

 $\rm CCSI^2$  has developed a standard solvent-based  $\rm CO_2$  capture system modeling framework with fundamental, multi-hierarchical characterization that will be used by the international  $\rm CO_2$  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  $CO_2$  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 Solvent Configurations; Lawrence Livermore National Laboratory—Device Scale Advanced Manufacturing; Oak Ridge National Laboratory—Intensified Packed Column Design; 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 | Oak Ridge National Laboratory | University of Kentucky | University of Texas at Austin | West Virginia University University of Notre Dame | University of Pittsburgh | University of Toledo | Carnegie Mellon University

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