the ENERGY lab

R&D FACTS

Computational Science

Carbon Capture Simulation Initiative

Description

The Carbon Capture Simulation Initiative (CCSI) is a partnership among national laboratories, industry, and academic institutions that will develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies in power plants from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. The CCSI Toolset will provide end users in industry with a comprehensive, integrated suite of scientifically validated models, with uncertainty quantification, optimization, risk analysis and decision making capabilities in order to increase confidence in designs, reducing the risk associated with incorporating multiple innovative technologies into new carbon capture solutions. The scientific underpinnings encoded into the suite of models will also ensure that learning will be maximized from successive technology generations.

Goals and Objectives

The CCSI Toolset will accelerate the development and deployment cycle for bringing new Carbon Capture and Storage (CCS) technologies to market in several important ways:

- Promising concepts will be more quickly identified through rapid computational screening of devices and processes.
- The time to design and troubleshoot new devices and processes will be reduced through science-based optimal designs.
- The technical risk in taking technology from laboratory-scale to commercial-scale will be more accurately quantified.
- The deployment costs will be stabilized more quickly by replacing some of the physical operational tests with virtual power plant simulations.

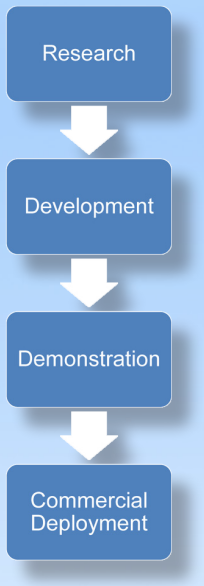
While the ultimate goal of the CCSI is to deliver a toolset that can simulate a broad set of new carbon capture technologies from laboratory-scale to full commercial-scale, the project scope during the first five years will focus on methods applicable to PC power plants, which generate nearly half the electricity in the United States and will emit 95% of the coal-based CO_2 between 2010 and 2035. Three Industrial Challenge Problems will be used to demonstrate the capabilities of the CCSI toolset: post-combustion capture by solid sorbents and advanced solvents, and oxy-combustion.

CCSI
Carbon Capture Simulation Initiative

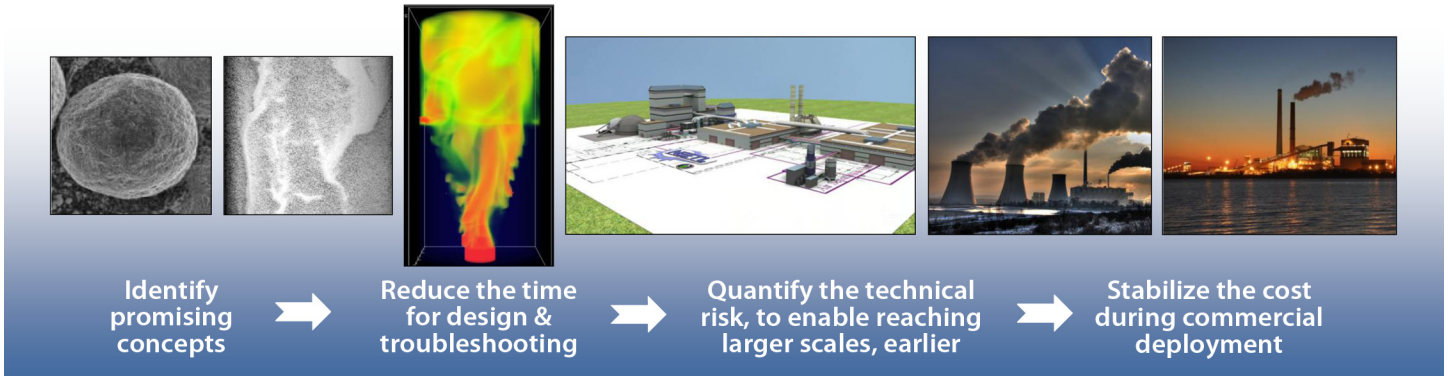
CONTACTS

David Miller
CCSI Technical Team Lead
Computational Science Division
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-6550
david.miller@netl.doe.gov

Madhava Syamlal
CCSI Director
Computational and Basic Sciences
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4685
madhava.syamlal@netl.doe.gov



By following these steps, CCSI will deliver a toolset that can simulate a broad set of new carbon capture technologies from laboratory-scale to full commercial-scale.



This model portrays the critical steps of the CCSI Toolset, which will increase confidence in designs and accelerate commercialization of innovative technologies for carbon capture.

Technical Approach

The CCSI project will leverage and support the Department of Energy's National Energy Technology Laboratory (DOE/NETL) Carbon Capture Simulation Research, Development, and Demonstration (RD&D) Program, an approximately $2 billion effort for FY11 through FY15. Data from CCS RD&D pilot and demonstration scale projects will be used to validate the CCSI methodology. In partnership with industry, the CCSI Toolset will be applied to reduce the scale-up risk associated with carbon capture technologies.

To address the three Industrial Challenge Problems, the CCSI Research and Development plan is organized around the following Focus Areas. The *Physicochemical Modeling and Simulation Focus Area* addresses multi-scale modeling, process synthesis and design, and process control for carbon capture technologies. The *Analysis & Software Focus Area* addresses the decision making framework to enable quantification of technical and economic risk, which will accelerate the scale-up and commercialization processes. The *Industrial Applications Focus Area* will define the detailed requirements for the industrial challenge problems, review and evaluate the results of the industrial challenge problems, and promote industry participation within CCSI. The Focus Areas consist of a total of 10 task sets, nine of which are led by a senior researcher from one of the five national labs. The tenth task set is led by one of CCSI's industrial partners.

As the CCSI Toolset is developed, it will undergo reviews by an Industry Advisory Board (IAB) semi-annually and a scientific peer review every 18 months. The IAB will ensure that the project is effectively addressing industry-relevant barriers to scale-up and commercialization, while the scientific peer reviews will ensure the quality of the scientific underpinnings of the models, tools, and approaches. To train current and future engineers in the use of the CCSI Toolset, summer schools will be held for industry practitioners, postdocs, and graduate students beginning in the third year of the project.

Benefits

Over five years, CCSI will develop an integrated, validated suite of models and computational tools for accelerating the development and deployment of carbon capture technology. The CCSI Toolset will be used during the scale-up of carbon capture processes to assess and mitigate technical and financial risks, to improve designs, and to shorten the design cycle. This will support decision making to move to larger scales, more quickly and with better designs, thereby considerably reducing the cost and time required for the commercialization of carbon capture technology. The CCSI Toolset will be released periodically to the CCSI industrial partners during the project and will target computer systems readily accessible by industry in 2015. The CCSI Toolset will be used by power generators for evaluating technical risk of scale-up, and by equipment manufacturers for screening and improving designs.

A Partnership for Success

The CCSI project is led by NETL and leverages the DOE national laboratories' core strengths in modeling and simulation, bringing together the best capabilities at NETL, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and Pacific Northwest National Laboratory. The CCSI's industrial partners provide representation from the power generation industry and the power equipment manufacturers. The initial industrial partners are ADA Environmental Solutions, Alstom Power, Ameren, Babcock Power, Babcock & Wilcox, Chevron, the Electric Power Research Institute, Eastman, Fluor, General Electric, Ramgen Power Systems, and Southern Company. The CCSI's academic participants (Carnegie Mellon University, the University of Pittsburgh, Virginia Tech, Penn State University, Princeton University, and West Virginia University) bring unparalleled expertise in multiphase flow reactors, combustion, process synthesis and optimization, planning and scheduling, and process control techniques for energy processes.

R&D156, April 2011