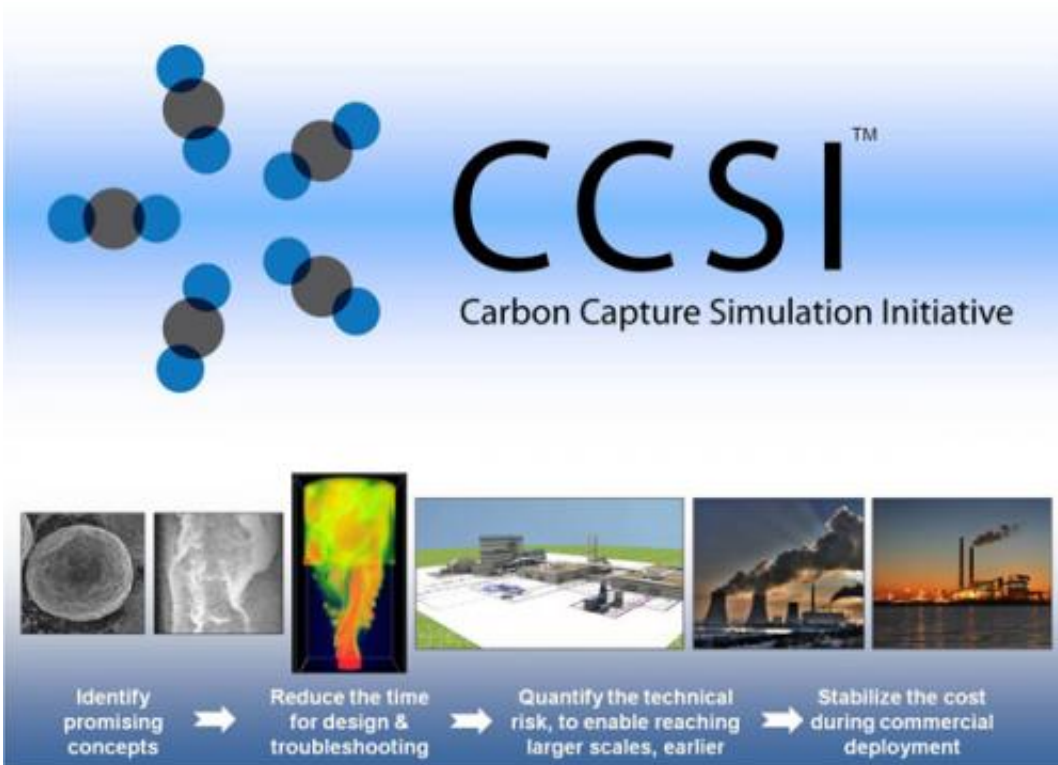


# Computer scientists developing tools to reduce greenhouse gases at the source

February 1 2013, by Jon Bashor



Despite advances in alternative energy sources, the United States will continue to rely on coal-fired power plants to generate much of the nation's electricity for the next 20 years or more. While coal is an economically viable fuel, its environmental cost is high—in 2011, coal accounted for 34 percent of the energy-related carbon dioxide (CO<sub>2</sub>)

emissions in the United States.

This is why a U.S. Department of Energy project, called the Carbon Capture Simulation Initiative (CCSI), is bringing together America's national laboratories, industry and academic institutions, to develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies in power plants.

As part of this collaboration, computational researchers at Lawrence Berkeley National Laboratory (Berkeley Lab) are playing key roles in the development of the computational tools. This past October, CCSI released their first set of tools and models at a meeting with representatives from the 19 companies that are currently participating on its industry advisory board.

"This pre-release, a year ahead of the originally planned first release, is the result of intense industry interest in getting early access to the tools and the phenomenal progress of the CCSI technical team," DOE's National Energy Technology Laboratory (NETL) Director Anthony Cugini wrote in a letter to Energy Department Secretary Stephen Chu. "These initial components of the CCSI toolset provide new models and computational capabilities that will accelerate the commercial development of carbon capture technologies and, really, an incredibly broad range of technology development in general—power, refining, chemicals production, gas production to name a few."

Because carbon capture systems are not yet required at any of the 600 plus plants across the country, CCSI works closely with industry to make the tools easier to adapt to existing design technologies. These tools would make it easier for utility companies to meet such requirements if and when they are enacted, and could help companies doing business in countries where controls are already in place. "CCSI brings together the

best capabilities in scientific [modeling and simulation](#) at our national laboratories, universities, and industry, to help industry address this unprecedented challenge at low cost, in less time," said Madhava Syamlal (NETL), Technical Director of the CCSI project, which is led by NETL.

### **Speeding up deployment of carbon capture technologies**

The broad goal of CCSI is to develop computational tools that will be used to accelerate the commercial development of advanced carbon capture technology. This includes (1) enabling promising concepts to be more quickly identified through rapid computational screening of devices and processes; (2) reducing the time to design and troubleshoot new devices and processes; (3) quantifying the technical risk in taking technology from laboratory scale to commercial scale; and (4) stabilizing deployment costs more quickly by replacing some of the physical operational tests with virtual power plant simulations. "The CCSI computational tools are delivering new capabilities for integrating multi-scale modeling, optimization and uncertainty quantification, which will significantly impact the way carbon capture processes are developed," said David Miller of NETL, technical lead of CCSI. "These tools will ultimately enable smarter, more focused pilot and demonstration scale projects."

"One of the goals is to accelerate the time needed to deploy carbon capture systems at [coal-fired power plants](#), but it's almost like walking a tightrope," said Deb Agarwal, head of the Advanced Computing for Science (ACS) Department and Berkeley Lab's CCSI lead for framework integration. "The corporations don't have a lot of incentive to invest in this area yet, but they will need to be able to ramp up quickly if such systems are required."

When completed, the CCSI Toolset will provide industry users with a

comprehensive, integrated suite of scientifically validated models that enable optimization of design, assessment of uncertainty, and understanding of risks to support decision making capabilities. This set will also give them increased confidence in designs and reduce the risk associated with incorporating multiple innovative technologies into new carbon capture solutions.

The recent Toolset release included a number of integrated applications consisting of CCSI tools and commercial software. Paolo Calafiura leads the software engineering team of Keith Beattie, Abdelilah Essiari, Sarah Poon, and David Robertson, as well as collaborators Greg Pope (LNNL) and Tim Carlson (PNNL). They are implementing the CCSI web portal ([www.acceleratecarboncapture.org](http://www.acceleratecarboncapture.org)) and software build, testing, and release processes. This first CCSI software release contained 19 new software packages and models, and the LBNL team orchestrated the testing of the manuals, tutorials, installers, and software and accomplished this on a tight schedule (six weeks) and on time.

For example, John Eslick at NETL and Jim Leek (LLNL) developed a library called "AspenSinter," which is used to integrate process models or flow sheets using AspenTech process modeling and flow sheet applications with the CCSI software framework. This has allowed the team to efficiently run and analyze half a million AspenTech simulations.

Meanwhile, Joshua Boverhof of CRD's Advanced Computing for Science Department developed the Turbine Science Gateway (TSG), a code for running the AspenTech process simulation applications in parallel on cloud computing systems, clusters, or on standalone machines. The TSG implements the parallel simulations needed by uncertainty quantification and optimization. Boverhof incorporated an auto-scaling component, allowing TSG to take advantage of lower-cost, on-demand resources at Amazon Web Services to run tens of thousands

of simulations together. He recently won honorable mention for TSG in a competition sponsored by Amazon.

Realizing the potential of CCSI depends on having an integrated carbon capture simulation environment that enables multi-scale simulations, uncertainty quantification, decision support, and optimization, all to interact, share data, and share results. In talking with industry partners, Agarwal said, "Many parts of the process are done separately, with very little carryover or connectivity, which can affect the time it takes to design a process. By integrating the steps, feedback can help quantify uncertainties in simulations and lead to improved tools." LBNL is the lead institution on the integration framework, data model, and data management development. Dan Gunter and Doug Olson of LBNL led the data model development to define the data interchange and storage formats.

An area where industrial researchers could benefit from CCSI modeling is in identifying promising adsorber materials—used in an adsorber designed to capture CO<sub>2</sub> molecules before the flue gas exits a power plant through a smokestack. Ideally, this chemical sponge would be able to continuously remove CO<sub>2</sub> from the plant's emissions and capture it. In addition to CO<sub>2</sub>, the adsorber would also need to handle the water vapor in the flue gas. A group of materials known as zeolites appear promising for this application, but the current challenge is to identify the one that works best at the lowest cost. To do this the CCSI team is tapping into the materials database created by DOE's Energy Frontier Research Centers, including the Center for Nanoscale Control of Geologic Carbon led by Berkeley Lab. Berend Smit, Maciej Haranczyk, Jihan Kim, Mahmoud Forrest Abouelnasr, and Kuldeep Jariwala have developed the calculations needed to help identify promising materials. The resulting database has been connected to the CCSI tools through the integration framework.

Other labs collaborating on CCSI are National Energy Technology (lead), Pacific Northwest, Los Alamos, and Lawrence Livermore national laboratories. Funding is currently provided through the Crosscutting Research Program of the U.S. Department of Energy's Office of Fossil Energy. The project was started with funding under the American Reinvestment and Recovery Act (ARRA).

This is why a U.S. Department of Energy project, called the Carbon Capture Simulation Initiative (CCSI), is bringing together America's national laboratories, industry and academic institutions, to develop and deploy state-of-the-art computational modeling and [simulation tools](#) to accelerate the commercialization of carbon capture technologies in power plants.

As part of this collaboration, computational researchers at Lawrence Berkeley National Laboratory (Berkeley Lab) are playing key roles in the management of the project and development of the computational tools. This past October, CCSI released their first set of tools and models at a meeting with representatives from the 19 companies that are currently participating on its industry advisory board.

"This pre-release, a year ahead of the originally planned first release, is the result of intense industry interest in getting early access to the tools and the phenomenal progress of the CCSI technical team," DOE's National Energy Technology Laboratory (NETL) Director Anthony Cugini wrote in a letter to Energy Department Secretary Stephen Chu. "These initial components of the CCSI toolset provide new models and computational capabilities that will accelerate the commercial development of carbon capture technologies and, really, an incredibly broad range of technology development in general—power, refining, chemicals production, gas production to name a few."

Because [carbon capture](#) systems are not yet required at any of the 600

plus plants across the country, CCSI works closely with industry to make the tools easier to adapt to existing design technologies. These tools would make it easier for utility companies to meet such requirements if and when they are enacted, and could help companies doing business in countries where controls are already in place.

Provided by US Department of Energy

Citation: Computer scientists developing tools to reduce greenhouse gases at the source (2013, February 1) retrieved 23 April 2024 from <https://phys.org/news/2013-02-scientists-tools-greenhouse-gases-source.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.