

CCSI™

Carbon Capture Simulation Initiative

First Year Successes

February 1, 2011 – January 31, 2012



Lawrence Livermore
National Laboratory



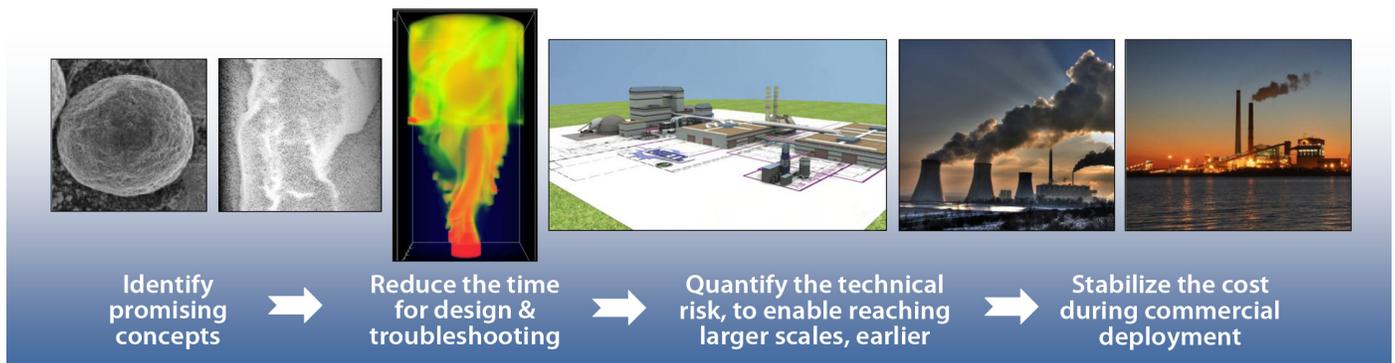
U.S. DEPARTMENT OF
ENERGY

The Challenge

The traditional pathway from discovery to commercialization of energy technologies usually takes two to three decades, but there is an urgent need to accelerate the development of carbon capture technologies. President Obama, in a February 2010 memorandum, charged a Carbon Capture and Storage (CCS) Task Force to overcome the barriers to widespread, cost-effective deployment of CCS within 10 years. In setting a goal to bring 5–10 commercial demonstration projects online by 2016, the President further stated: “If we can develop the technology to capture the carbon pollution released by coal, it can create jobs and provide energy well into the future.” Carbon Capture and Storage involves capturing carbon dioxide (CO₂) from large point sources such as power plants and industrial facilities, and storing it in ways that prevent the greenhouse gas from entering the atmosphere.

U.S. Department of Energy - Fossil Energy Response to the Challenge

Carbon Capture, Utilization, and Storage is a key component in national efforts to curb climate change. Meeting the President's goal to begin deployment of carbon capture technology within 10 years will require the development of new approaches to quickly scale up laboratory concepts for a power plant. Consequently, the U.S. Department of Energy (DOE) through its National Energy Technology Laboratory (NETL), has identified the Carbon Capture Simulation Initiative (CCSI) as a new approach to take carbon capture concepts from the laboratory to the power plant quickly and at low cost and risk, complementing several laboratory and pilot-scale projects supported by DOE. The aerospace and automotive industries have recently demonstrated that simulations can be used to accelerate technology development. CCSI will combine recent advances in simulation technology to develop a science-based capability to assess and mitigate the risk of scaling up carbon capture technologies and reduce development cost and time.



The primary goal of CCSI is to provide technology developers and plant operators with a validated suite of models and simulation tools to enable the rapid development and deployment of new carbon capture technologies.

The project targets the development of capabilities applicable to post-combustion carbon capture that are expected to have the greatest immediate impact on U.S. pulverized coal power plants—which currently generate nearly 40 percent of the nation's electricity and are expected to emit 95 percent of the CO₂ from United States' coal-based power plants between 2010 and 2030. NETL assembled a team from DOE national laboratories and universities to develop the simulation technology. The initiative has attracted a group of active industrial partners who ensure that CCSI products are of immediate interest to industry and can be quickly adopted.

Academia Partners

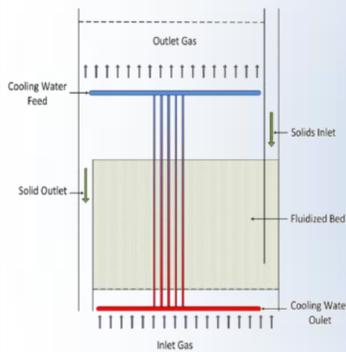
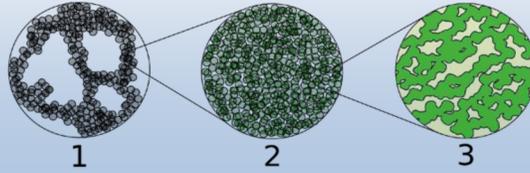


Industry Partners



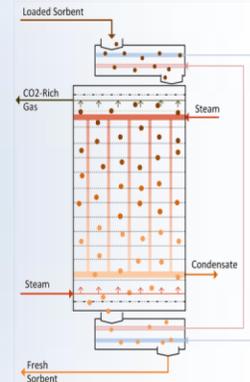
Sorbent Kinetics Model that Predicts Competitive Uptake and Release of CO₂.

Flue gas contains significant moisture that strongly influences the performance of a carbon capture system both beneficially and adversely. A kinetic model was developed to provide process developers with a more complete understanding of the behavior of sorbent particles to enable better designs.



Detailed Process Models for Bubbling Fluidized Bed and Moving Bed Reactors for Solid Sorbent Capture Systems.

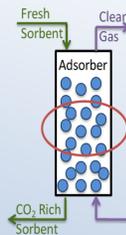
These models enable evaluation of potential carbon capture processes using commercially relevant equipment configurations. Prior to CCSI, models of these systems were not available for commercial process simulators.



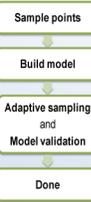
ALAMO, a Software Tool That Enables the Design of Optimal Capture Processes.

ALAMO develops fast process models required for advanced optimization-based process synthesis. This allows designers to more easily find the best process configuration for potential carbon capture systems, while considering a variety of trade-offs.

Detailed model developed in commercial process simulation tool

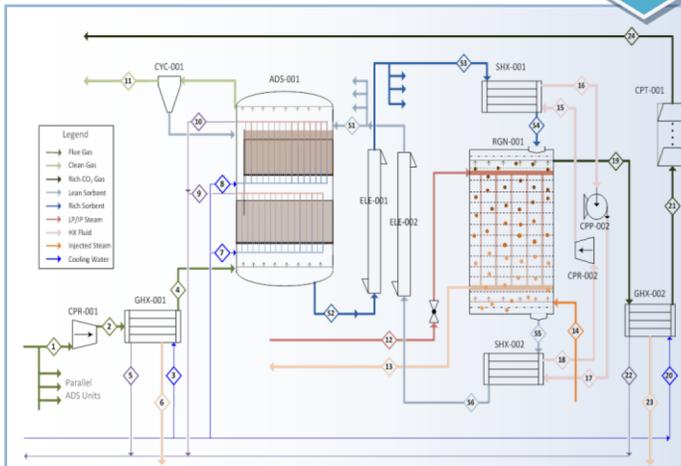
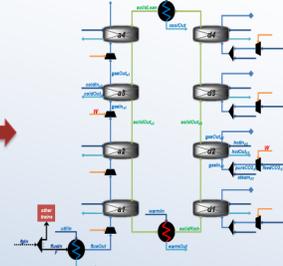


Develop Algebraic ROM



$f(x)$

Formulate and solve superstructure to determine optimal process configuration

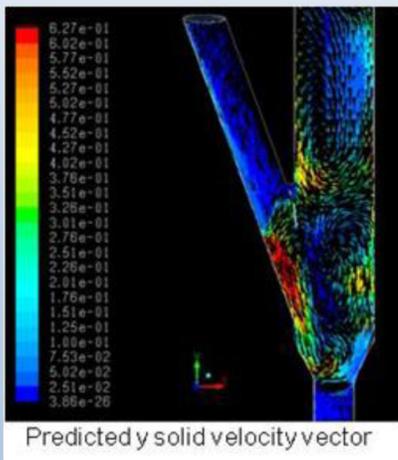


Simulation-based Optimization Framework for The Design of a Complete Carbon Capture and Compression System Integrated with a Pulverized Coal Power Plant.

The framework has been used to complete the most comprehensive design and systems analysis to date. It will be used as the basis for demonstrating future design and analysis developed under CCSI.

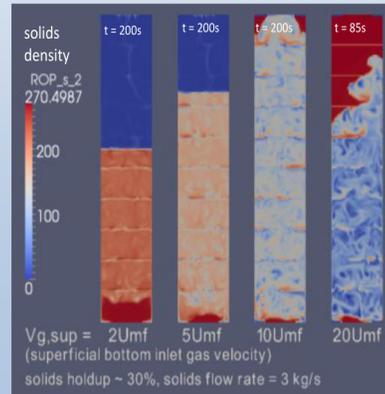
Simulation and Validation of an Actual Pilot-scale (1kwe) Solid Sorbent Process Model for a Post-combustion Capture Technology.

Computational fluid dynamics simulations of an amine-based solid sorbent capture process were validated against process data taken with real flue gas. Validation demonstrates that these models can reliably predict the performance of these types of systems.



Models of Large-scale (650 Mwe) CCS Adsorber and Regenerator Using the Open-source Code MFIX.

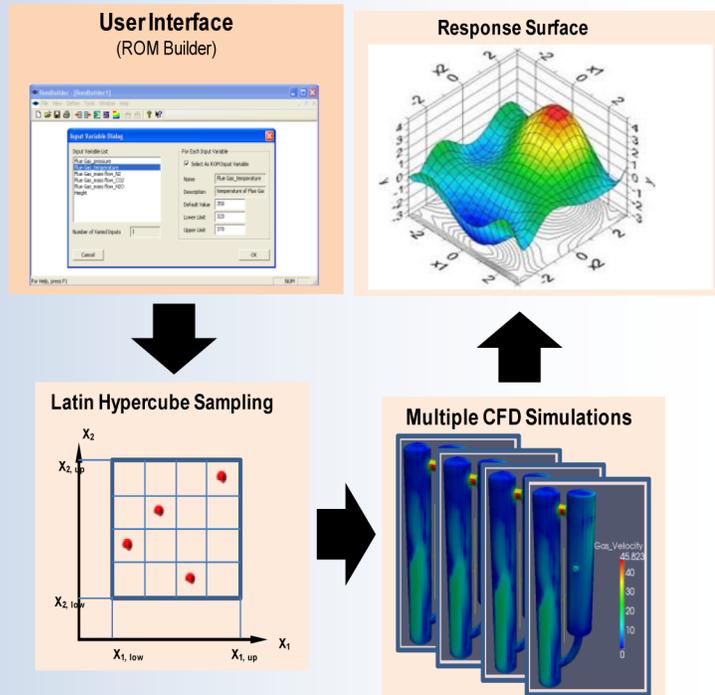
These models demonstrate that simulations of large-scale capture devices can be successfully carried out. They comprise a set of “starter models” that industry can use to develop their own simulations. These models provide insight into the solid-sorbent simulation process and can also be used to improve the design of carbon capture systems by identifying issues that may emerge at large-scale prior to construction of actual equipment, thus saving significant time and money during scale-up.



An Automated Workflow for The Development of Reduced Order Models (ROM) from MFIX.

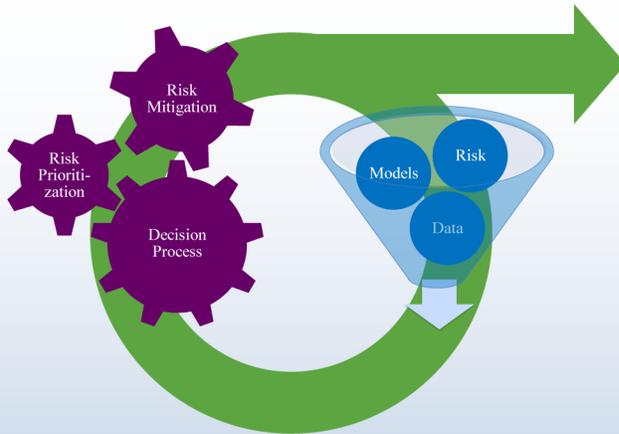
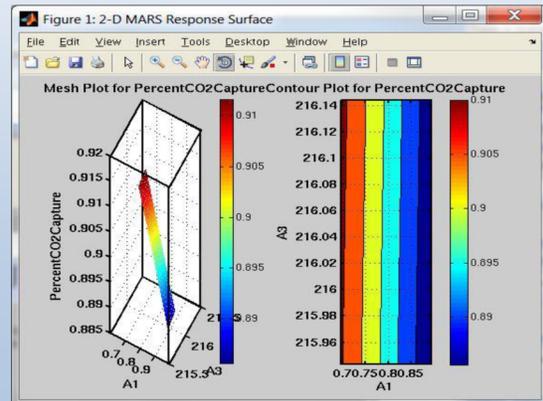
In order to effectively enable high fidelity CFD simulations to be used for uncertainty quantification and optimization, it is often necessary to develop ROMs.

The ROM tools that the CCSI has developed and demonstrated are focused on enabling interoperability so that the capabilities of the software packages can be leveraged across the entire CCSI Toolset. Methods of integration include the use of ROMs for transferring information from one scale to another and preserving information generated at different scales.



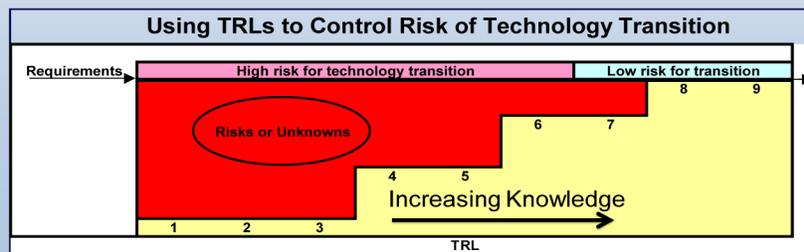
Uncertainty Quantification Applied to Process Simulations.

PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration), originally developed by LLNL for NNSA, was linked to windows-based process simulators. This capability is an essential first step for quantifying and propagating model and parameter uncertainty across simulation scales. The capability was demonstrated by evaluating the uncertainties associated with a carbon capture process based on an aqueous monoethanolamine solvent. An initial set of capabilities for UQ analysis was developed (parameter screening, response surface analysis, quantitative sensitivity analysis, and parameter estimation).



Demonstration of a Risk Analysis and Decision Making Methodology.

The prototype software tool quantifies the risk of a hypothetical investment in carbon capture technology for a 650 MWe pulverized coal power plant. It incorporates knowledge from the whole range of models used across CCSI combined with uncertainty quantification to enable risk prioritization and mitigation. The framework uses qualitative risk factors, concepts of probabilistic decision-making, and risk contributors based on a modified technology readiness level concept.



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