Computational Toolset for Accelerating Carbon Capture Technology Development

Madhava Syamlal

National Energy Technology Laboratory (NETL), Morgantown, WV 26505, USA

Corresponding author: madhava.syamlal@netl.doe.gov

Summary

The Carbon Capture Simulation Initiative (CCSI) is a partnership among national laboratories, industry and academic institutions led by NETL that is developing computational modeling and simulation tools for accelerating the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. 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. The CCSI Toolset consists of a comprehensive, integrated suite of scientifically validated models, with uncertainty quantification, optimization, risk analysis and decision making capabilities. The CCSI Toolset incorporates commercial and open-source software currently in use by industry and new software tools developed to fill technology gaps identified during the execution of the project. The CCSI Toolset will (1) enable promising concepts to be more quickly identified through rapid computational screening of devices and processes; (2) reduce the time to design and troubleshoot new devices and processes; (3) quantify the technical risk in taking technology from laboratory-scale to commercial-scale; and (4) stabilize deployment costs more quickly by replacing some of the physical operational tests with virtual power plant simulations. The CCSI Toolset uses a multi-scale approach for modeling CO_2 capture processes, including models of particle/film-scale reaction kinetics, computational fluid dynamic models of capture reactors, and steady and dynamic models of capture processes. Reduced order models are used for transferring information between scales and for enabling tractable process synthesis calculations. The models are validated with data from lab and pilot-scale experiments, and the uncertainty in the models is systematically quantified and propagated across scales. The modeling results are used for determining optimal reactor configurations and operating conditions. This presentation will give an over view of the current status of CCSI Toolset.