Predicting scale-up performance using validated CFD model with quantitative confidence

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The Carbon Capture Simulation Initiative (CCSI), a partnership among DOE national laboratories, industry, and universities, is developing a suite of multi-scale modeling and simulation tools aimed at dramatically accelerating the development and deployment of post-combustion carbon capture technologies. As a candidate for large scale post-combustion \( \text{CO}_2 \) capture, solid sorbent-based capture system is attracting researchers’ attention with the potential to reduce energy consumption, improve regeneration, enable greater capacity, and offer selectivity as well as ease of handling. Even though multiple laboratory or pilot scale facilities exist for different carbon capture demonstration projects, the ability to quantitatively assess and predict capture performance and capacity at the plant scale is a critical barrier to their commercial scale deployment.

In CCSI, high fidelity computational fluid dynamics (CFD) simulations are used to simulate the device-scale complex multiphase reactive flow phenomena to evaluate the specific reactor design and to provide device-scale reduced order models for plant-level system synthesis simulations. The heart of the solid sorbent-based capture system is typically a fluidized bed reactor with specific geometry and designed flow regime. Because of the infeasibility of designing and conducting validation experiments on the full-scale systems, we quantify the device-scale prediction confidence for plant scale capture with available laboratory/pilot scale and separate effect experiments following a rigorously designed hierarchical calibration and validation process.

In this study, the complex solid sorbent carbon capture system is divided into several tiers of unit problems with progressively increasing physical coupling/complexity and increasing length scales. The lowest length-scale on the device-level validation hierarchy is comprised of the unit problems encountered in a typical fluidized adsorber, where each unit problem represents an important physical phenomenon. For the currently investigated bubbling fluidized bed system, the important physical phenomena, i.e., unit problems, are identified as (1) flow hydrodynamics in a bubbling fluidized bed; (2) reaction kinetics occurring at the particle scale; and (3) heat transfer,
which are expected to be significant in the adsorber due to the exothermic nature of the reaction and the various cooling mechanisms employed. From a modeling perspective, each unit problem can be viewed as a set of models, and suitable choices for each model and its parameter ranges will be based on existing knowledge or, if possible, the calibrated posterior distribution from the simpler unit problem. For example, in the bubbling fluidized bed unit problem, several options are available for modeling the gas drag force experienced by the fluidized particles. As some model choices are expected to perform better than others, the identification of the best available models and their parameters are part of the CCSI validation activity. On the experimental side, laboratory scale separate-effect and integrated effect experiments have been performed at the NETL C2U reactor for the unit problems described above with statistically designed operating parameters. The C2U device-scale measurements for the decoupled (cold flow, flow + heat transfer) unit problems are used to progressively calibrate the modeling parameters with a general Bayesian calibration/ model assessment methodology using a Bayesian Smoothing Spline (BSS) ANOVA emulator. The BSS-ANOVA tool takes as input experimental results in the form of input settings and resulting output(s), along with simulation results in the form of parameter and input settings and resulting output(s). It then performs a Bayesian calibration to find a posterior distribution of parameter settings for the simulator that allows it to best reproduce the experimental data. Once the Bayesian calibration is done on a simpler unit problem, the posterior distributions of the parameter set are passed along as the prior distribution for the unit problems at the next level of physical complexity.

With the calibrated posterior parameter distributions from the couple unit problems and the filtered models, we perform the fully coupled multiphase reactive flow CFD simulations at the next scale, i.e., the 1MW pilot-scale adsorber, and quantify the predictive confidence level based on knowledge obtained from the C2U validation and calibration process. A fully coupled multiphase flow CFD model with chemical reaction, energy, and species transport is developed to solve for the spatial and temporal dependent flow, temperature, and species distributions within the entire reactor, and to predict the device’s overall performance on CO2 capture. In the meantime, using a large amount of simulation cases with model input parameters covering the posterior distributions resulting from the calibration of the C2U unit problems, a quantified confidence level can be derived for each operating condition.