CFD model validation of a small scale Carbon Capture Unit

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A hierarchical validation framework has been developed by the Carbon Capture Simulation Initiative (CCSI) team for predicting the device-scale CO_2 adsorption utilizing solid sorbent with a multi-phase computational fluid dynamics (CFD) model. CCSI is a partnership among U.S. national labs, academia and industry that is developing computational tools needed for taking carbon capture concepts from the laboratory to the power plant quickly and at low cost and risk. In the CCSI hierarchical validation framework, unit problems with increasing level of physical complexities are used as the building blocks for progressive model validation, parameter calibration, and uncertainty quantification. It has been demonstrated that the CFD model can be used to accurately capture the flow hydrodynamics and CO_2 capture performance of a bubbling fluidized bed adsorber of a lab-scale Carbon Capture Unit (C2U). However, the simulations also revealed that special attention is required to validate the reaction kinetics developed from thermo-gravimetric analysis (TGA) data due to the large difference in the time scales between TGA and C2U experiments. For this reason, a small-scale CO_2 Capture Unit (mini-C2U) was recently built at the National Energy Technology Laboratory to validate the CO_2 adsorption kinetics. Tests of both cold and reacting flow under different conditions are being conducted using different solid sorbents. The CCSI validation framework will be applied to the mini-C2U with special focus on CO2 capture kinetics and its coupling with the flow hydrodynamics. The validated model will be used to simulate and help to optimize the 1MW pilot-scale reactor being built by an industrial collaborator.