CCSI CFD Models

Since the key capture adsorption/absorption reaction occurs at the device scale, high fidelity CFD models at this scale can help the design engineers in trouble shooting and screening the various design factors for desired device performance.

This product bundle contains all the device scale CFD models developed in the course of CCSI project, and they include the coupled reactive gas particle flow model for the 1MWe sorbent-based adsorber, CFD models for the decoupled and coupled bench-scale C2U cases in order to build a hierarchical calibration and validation framework for quantifying the predictive confidence for systems yet to be built, gas-particle subgrid filtered models with and without the presence of heat exchanger tubes to enable geometric upscaling, as well as particle attrition models for predicting particle side degradation. It also contains the solvent-relevant CFD models and modules developed by the CCSI team in an effort to predict the device-scale behaviors for a solvent-based capture system.

The CFD models are categorized as follows:

Sorbent-based capture:

1. CCSI Validation and Uncertainty Quantification Hierarchy for CFD Models.
2. Device Scale CFD Models for Sorbent: This product suite first contains the full scale high fidelity CFD model files for the adsorber unit of the 1MWe solid sorbent carbon capture system. This product also includes all the bench-scale C2U models from cold flow, non-reactive hot flow to fully coupled reactive flow in an effort to build up the validation and calibration hierarchy. It applies hierarchical model calibration and validation procedures in predicting device-scale CO2 adsorption. Users are suggested to follow the product installation guide to install the models and run the simulations, and to consult the corresponding CCSI milestone report [Ref.] for the detailed uncertainty quantification procedures.

3. Subgrid Filtered Models for Geometric Upscaling: Because of the extreme disparity between the particle size and the overall dimension of the adsorber, explicit resolving the small-scale flow structures and heat transfer cylinders is computationally prohibitive. To enable accurate macroscopic predictions using coarse-grid simulations, various subgrid filtered models are developed by CCSI. These filtered models account for the presence of unresolved physics and geometry via constitutive subgrid equations, and they include: a.) cylinder-suspension drag [1], b) cylinder-suspension heat transfer [2], and c) gas-particle interphase drag in MFIX [3]. The cylinder-based models are valid for an array of horizontal tubes immersed in the flow. In the simulations, the cylinders are replaced by an effective stationary porous media, occupying the same volume as the cylinders and the drag [1] and heat transfer [2] are modified through source terms added to the governing equations.

4. CCSI Attrition and Pulverization Model: Particle attrition is frequently encountered during the processing and handling of mesoporous particles in chemical processing, where the particles suffer progressive loss of material as a result of collisions and friction [Hutchings, 1993]. In fluidized bed reactors, particle size reduction due to attrition can result in

agglomeration and poor fluidization [Pougatch et al., 2010], and the generation of fine debris may further constitute health hazards, leading to environmental pollution [Jørgensen et al., 2005]. A discrete element method (DEM)-based attrition model was developed to investigate the attrition of initially monodispersed solid particles in a jet cup. Particle size reduction due to chipping and abrasive wear from particle-particle and particle-wall interactions were considered and explicitly implemented into the simulation. The attrition models can be used to study the effects of operational factors, such as jet velocity, particle size, solid density, and jet cup design on the attrition propensity.

The Coal Pulverization Model, which was developed by extending the CCSI DEM-based modeling capability, is also included in this product category.

Solvent-based capture:

5. A Validation Hierarchy for CFD Models of Solvent-based Carbon Capture Systems.
6. Simulating Liquid Film Flow over an Inclined Plate: This product contains the CCSI developed capability in predicting interfacial and wetted areas and film thickness for liquid film flow over an inclined plate. VOF-based multiphase flow simulation is developed for film flow over an inclined plate. The model can be used to systematically study the effects of a wide range of parameters, including inlet cross section, flow rate, plate inclination angle, range of solvent properties, and contact angles on the flow characteristics. Based on results of rigorous and extensive simulations, scaling theory was also developed for interfacial and wetted areas and film thickness.
7. Wetted Wall Column (WWC) Models for Effective Mass Transfer and Reaction Parameters: This product suite contains the VOF-based CFD models for predicting the gas/solvent interactions in a wetted wall column experiment, and it includes WWC models on hydrodynamics, hydrodynamics with mass transfer, and finally hydrodynamics with mass transfer and absorption reactions. Both experimental and simulation conditions are statistically designed, and the BSS-ANNOVA-based calibration process is demonstrated in this product suite. The posterior distributions of effective mass transfer coefficient with quantified uncertainty for the WWC can be obtained for solvents with different physical and chemical properties. This product represents one of the unit problems in enabling an at-scale prediction for a solvent-based packed column absorber.