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Numerical modeling and uncertainty quantification of a bubbling fluidized bed with immersed horizontal tubes

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ABSTRACT

Within the field of computational fluid dynamics (CFD), uncertainty quantification (UQ) is becoming increasingly important. Reporting simulation results without uncertainties can be misleading and potentially dangerous. In this paper we considered an isothermal, non-reacting bubbling fluidized bed with immersed horizontal tubes as a test problem for implementing a CFD UQ framework. While all CFD model input parameters have some inherent uncertainties associated with them, we focused only on those that have been demonstrated as important in previous studies and are difficult to quantify. These include coefficients of restitution, friction angles, packed bed void fractions, and drag models. Statistical UQ techniques, including sensitivity analysis and Bayesian calibration, were used to analyze the system. The sensitivity analysis results suggested that the friction angles for solid-solid interactions and drag models had significant effects on bubble frequency and phase fraction. From the calibration procedure, a statistical response surface model (emulator) was developed to explore the state-space of the model parameters. The resulting posterior distributions of the model parameters identified low friction angles for solid-solid interactions and the Wen-Yu correlation for the drag model as the optimal model input parameters and values (i.e., values that could have plausibly reproduced the experimental results). The remaining parameters were found to be non-influential. These results are currently being implemented in simulations of a bench-scale carbon capture system.

1. Introduction

Fluidized beds are widely used in chemical engineering systems and processes (e.g., combustion, mixing, polymerization, and carbon capture) because of their high heat and mass transfer rates, uniform mixing, and continuous-operation abilities [1]. Their wide range of configurations and applications, and inherently complex behavior present many challenges to both experimental and computational researchers. In this paper, we investigate a bubbling fluidized bed with immersed horizontal heat transfer tubes, based on the experimental work of Kim et al. [2], with emphasis on uncertainty quantification (UQ).

Compared to traditional single-phase flows, numerical modeling of multiphase flows requires additional mathematical models, such as drag, granular temperature, turbulence, and friction models. These models have been developed based on empirical and theoretical constitutive relations. Consequently, results can vary significantly depending on the choice of models used. Furthermore, physical quantities, such as coefficients of restitution, friction angle, and packed bed void fraction, can be difficult to measure experimentally and are often chosen based on previous studies or without rationalization. Because there is no single correct choice for the aforementioned models and quantities, there exists an associated uncertainty for each choice. Identifying, quantifying, and reporting these uncertainties are essential for computational research to preserve the integrity of the results. When modeling unsteady complex systems like fluidized beds, uncertainty analysis becomes a necessity.

Statistical UQ techniques, such as sensitivity analysis and Bayesian calibration, can help quantify uncertainties in the system and make out-of-sample output predictions [3–6]. A sensitivity analysis quantifies the variation in output that is directly related to the uncertainty and variation in the model input parameters. This can identify important (and unimportant) model parameters, allowing for improved control and simplification of the model being assessed. Additionally, Bayesian calibration methods [7] can be implemented with statistical response surface models (emulators) that are capable of quickly approximating the system. Bayesian calibration uses Markov chain Monte Carlo methods to determine the optimal model parameter values (i.e., values that

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could have plausibly reproduced the experimental results). These approaches are used in this paper and are discussed in further detail in Section 4. There have been a few recent applications of UQ to multiphase systems [8,9]; however, the applications are sparse. We aim to expand the knowledge and use of UQ in the field of computational fluid dynamics (CFD) by considering the adsorber of a solid-sorbent carbon capture unit as part of the Department of Energy's (DOE's) Carbon Capture Simulation Initiative (CCSI).

CCSI aims to develop computational modeling and statistical tools to evaluate and quantify the performance, risk, and uncertainty of carbon capture technologies. Performing UQ analyses on full-scale CFD models is impractical due to the large number of required simulations. Instead, a verification and validation (V&V) hierarchy [10] has been developed to effectively reduce the complex system to smaller, simpler unit problems based on physics and length scales. The conceptual carbon capture system developed by CCSI is a post-combustion solid-sorbent system composed of two main components: an adsorber and regenerator, which can be further broken down into their unit problems: hydrodynamics, heat transfer, and reaction kinetics. This study investigates the hydrodynamics of the adsorber through a simplified bubbling fluidized bed model.

In this paper, we outline our framework for simulating and evaluating uncertainties in a fluidized bubbling bed. The numerical methods and CFD mathematical models used throughout this study are reviewed in Section 2. The experimental and computational system setups are described in Section 3. Section 4 outlines the statistical methods for sensitivity analysis, uncertainty quantification, and Bayesian calibration. The results are discussed in Section 5 and the concluding remarks are presented in Section 6.

2. Numerical methods

In this study we used the DOE's open source CFD code, Multiphase Flow with Interphase eXchanges (MFIX) [11], to investigate the hydrodynamics of a bubbling fluidized bed. Many CFD software packages and codes are capable of simulating multiphase flow, such as ANSYS Fluent, Barracuda®, MFIX, and OpenFOAM®; however, MFIX was chosen for this study because it has been developed explicitly for solving multiphase systems and is open source. The ability to view and modify the source code, makes MFIX ideal for our research purposes. Additionally, MFIX has been used to simulate numerous multiphase and multiphysics systems (e.g., circulating and bubbling fluidized beds, combustion reactors, and chemical vapor depositors) [12–17] and is continuously going through systematic V&V.

Multiphase flow simulations generally fall into one of two classifications: Eulerian-Eulerian (E-E) or Eulerian-Lagrangian (E-L) frameworks. In the E-E approach, all phases are treated as interpenetrating continua. In two-phase flow, this simplifies to the two-fluid model (TFM), which is used in this study. In the E-L approach, fluid phases are treated as continua while solid phases are treated as discrete particles. Several methods for E-L exist and are commonly used in multiphase flow simulation, for example, discrete-element method (DEM), dense discrete-phase model (DDPM), and multiphase-particle-in-cell (MPPIC) method. Both modeling frameworks have been used to successfully simulate fluidized beds [12,16,18,19]. The DDPM was previously considered for the carbon capture system modeling of CCSI [20]; however, due to numerical stability issues and the computational expense of the DDPM, it was decided the TFM was more appropriate for our applications.

A summary of the equations used by MFIX for solving isothermal, non-reacting, two-phase flow can be found below. For a complete description of the equations implemented in MFIX, see Benyahia et al. [11]. GNU gfortran (4.4.2) and OpenMPI (1.4.2) were used to compile and parallelize the simulations, respectively. Intel Xeon E5-2680 CPUs (8 cores) took 2 days to simulate 60 s of the bubbling fluidized bed described in Section 3.

2.1. Governing equations

The continuity and momentum equations can be written for each phase as

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\right)=0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s\right)=0 \tag{2}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\boldsymbol{u}_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\boldsymbol{u}_g\right)=\nabla\cdot\boldsymbol{\tau}_g-\varepsilon_g\nabla p+\varepsilon_g\rho_g\boldsymbol{g}-\beta\left(\boldsymbol{u}_g-\boldsymbol{u}_s\right) \tag{3}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\boldsymbol{u}_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s\boldsymbol{u}_s\right)=\nabla\cdot\boldsymbol{\tau}_s-\varepsilon_s\nabla p+\varepsilon_s\rho_s\boldsymbol{g}+\beta\left(\boldsymbol{u}_g-\boldsymbol{u}_s\right), \tag{4}$$

where ε is phase fraction, ρ is density, $\boldsymbol{u}$ is velocity, $\boldsymbol{\tau}$ is stress, p is pressure, $\boldsymbol{g}$ is gravitational acceleration, β is the interphase momentum transfer coefficient, and subscripts g and s denote the gas and solid phases, respectively.

2.2. Kinetic theory

Solving the governing equations in the TFM requires appropriate closure relations to calculate the solids properties (e.g., viscosity and pressure). The Kinetic Theory of Granular Flow provides necessary closures by quantifying the energy in the solid-phase. This energy is proportional to the mean square of the solid-phase velocity and is referred to as the granular temperature (GT). The full partial differential equation for GT is written as

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\Theta\right)+\nabla\cdot\left(\varepsilon_s\rho_s\Theta\right)\boldsymbol{u}_s\right]=\boldsymbol{\tau}_s:\nabla\boldsymbol{u}_s-\nabla\cdot\boldsymbol{q}_\Theta-\gamma_\Theta+\Pi, \tag{5}$$

where Θ is granular temperature, $\boldsymbol{q}_\Theta$ is diffusive flux of granular energy, γ_Θ is granular energy dissipation, and Π is interphase exchange of granular energy [21]. Because solving the full GT partial differential equation can be computationally demanding, Syamlal [22] proposed an algebraic expression for GT that neglects convection and diffusion terms and retains the generation and dissipation terms [21]. These simplifications are only valid for dense-flow regimes. The algebraic expression for GT is

$$\Theta=\left\{\frac{-K_1\varepsilon_s\mathrm{tr}(D_s)+\sqrt{K_1^2\mathrm{tr}(D_s)\varepsilon_s^2+4K_4\varepsilon_s\left[K_2\mathrm{tr}(D_s)^2+2K_3\mathrm{tr}\left(D_s^2\right)\right]}}{2\varepsilon_sK_4}\right\}^2 \tag{6}$$

$$K_1=2(1+e_{ss})\rho_sg_0 \tag{7}$$

$$K_2=\frac{4d_s\rho_s(1+e_{ss})\varepsilon_sg_0}{e\sqrt{\pi}}-\frac{2}{3}K_3 \tag{8}$$

$$K_3=\frac{d_s\rho_s}{2}\left\{\frac{\sqrt{\pi}}{3(3-e_{ss})}\left[\frac{1}{2}(1+3e_{ss})+0.4(1+e_{ss})(3e_{ss}-1)\varepsilon_sg_0\right]+\frac{8\varepsilon_sg_0(1+e_{ss})}{5\sqrt{\pi}}\right\} \tag{9}$$

$$K_4=\frac{12\left(1-e_{ss}^2\right)\rho_sg_0}{d_s\sqrt{\pi}}, \tag{10}$$