Chemical Engineering Science 176 (2018) 409–420

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Verification, validation, and uncertainty quantification of a sub-grid model for heat transfer in gas-particle flows with immersed horizontal cylinders

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HIGHLIGHTS

- Model showed excellent transient and steady state behavior with verification cases.
- Large-scale validation agreed well with test cases, observing 100,000+ times speedup.
- Prediction intervals from bootstrapping and MATLAB's `nlpredi` were within ±20%.
- Simulated a fully-reacting 1 MW CO_2 adsorber, outperforming ad-hoc approaches.

ARTICLE INFO

Article history:
Received 10 July 2017
Received in revised form 21 September 2017
Accepted 12 November 2017
Available online 13 November 2017

Keywords:
Sub-grid
Multiphase
Heat transfer
Verification
Validation
Uncertainty quantification

ABSTRACT

In previous work we developed and implemented a sub-grid model for the efficient simulation of heat transfer in gas-particle flows around immersed horizontal cylinders. In this study we apply verification, validation, and uncertainty quantification methods to the developed model to rigorously examine its capabilities and limitations. Numerical verification with small, unit-cell problems shows excellent transient and steady-state behavior. Validation of a bubbling bed and a turbulent bed showed good agreement with high-resolution simulations. To quantify the error of the constitutive model predictions two methods were used to calculate confidence intervals, showing an error of approximately ±20%, well within the range of typical Nusselt number approximations. The sub-grid model was applied to a conceptual pilot-scale 1 MWe carbon capture reactor to compare with alternative modeling methods. Results show fair predictions of hydrodynamics, heat transfer, and carbon capture rates with significant savings in computational runtimes.

1. Introduction

Computational models have become ubiquitous in all science and engineering fields. The ongoing acceleration of computing technology fuels the demands for larger, more complex models. To maintain tractability in these simulations, efficient approximation models must be employed.

In the field of multiphase flows, computational models can be classified as either Eulerian-Eulerian (multi-fluid continuum models) or Eulerian-Lagrangian (discrete particles models). In either case accurately resolving the multiphase and multiphysics dynamics requires very fine grid/particle sizes, requiring high performance computer clusters and long run-times. To reduce time and resource requirements, many accelerated simulation methods have been developed, e.g., Energy Minimization Multi-Scale (EMMS) (Li, 1994, 1987), Coarse Grained Particle Methods (CGPM) (Lu et al., 2016, 2017; Nasato et al., 2015), and sub-grid filtering models (Smagorinsky, 1963; Igci et al., 2008; Sarkar et al., 2013; Lane et al., 2016). The EMMS model used a multi-scale, multi-regime approach to minimize the energy of the system to predict the interphase drag and the flow fields. This is typically combined with a coarse grid to expedite calculations. CGPMs use large meso-scale particles to represent clusters of micro-scale particles, reducing the total number of particles. Similar to the EMMS, new closure models for the drag, collisions, pressure, etc. are used to approximate the microscopic behavior. Sub-grid filtering methods are similar to both of the previous models. The flow fields for a coarse grid system are calculated using derived closure models for the physics of interest. The effects of these approximations varies based on the model and system but can result in significant time savings at the

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https://doi.org/10.1016/j.ces.2017.11.018
0009-2509/

expense of model accuracy. As such, rigorous verification, validation, and uncertainty quantification (VVUQ) methods should be applied to ensure the integrity of the physics remains.

Verification is the first step in evaluating a newly developed model. It is a check to ensure that the model is behaving properly, conforming to the physical and mathematical rules as intended. For computational models, this involves correct implementation of the logic and mathematical formulae and checking with known analytical solutions.

Once a model has been verified, it should then be applied to, and compared with experimental setups and results. This is the validation step and it provides critical feedback on the accuracy of the model with non-standard tests. To fully validate the model, the test cases should encompass the full spectrum of possible scenarios. This will result in a better understanding of the capabilities (and shortcomings) of the model.

Because mathematical models are only approximations of physical phenomena, there exists quantifiable deviations from analog physical experiments. These deviations can be unpredictable in nature and can be thought of as model uncertainties. Since it is often the case that these models are developed for use on systems without experimental data, it is imperative that the uncertainties are quantified and incorporated within the model. This process is known as uncertainty quantification (UQ). The field of UQ is rapidly growing and developing new techniques to address these issues (Bryant et al., 2015; Gramacy et al., 2014; Higham et al., 2013).

In this study we present a verification, validation, and basic uncertainty analysis for a multi-scale, multi-physics, multiphase, computational fluid dynamics (CFD) model developed in our previous work (Lane et al., 2016). The model is an algebraic Nusselt correlation for efficient simulation of heat transfer in large-scale gas-particle systems with immersed heating or cooling geometry (Lane et al., 2016). It was developed in collaboration with the Department of Energy as part of their Carbon Capture Simulation Initiative (CCSI) (Miller et al., 2014). As such, our focus is on reducing computation time of similar large-scale systems, e.g., fluidized and moving bed chemical reactors. However, the VVUQ methods presented are applicable to any modeling approach.

Because of the complexity of these models/systems, analytical solutions do not exists. Instead, we use small-domain units cells for verification, with similar high-resolution simulations for comparison. The model is then validated with two different fluidized bed systems, again, using high-resolution computational models in lieu of unavailable experimental data. Finally, using two statistical UQ approaches, the estimation error of the model is predicted for the range of the model. The methods presented in this paper advance the application of VVUQ to complex, computationally expensive CFD simulations and are generally applicable to general CFD modeling.

2. Numerical methods

The simulations presented in this study were solved using Multiphase Flow with Interphase eXchanges (MFIX), the open source, multiphase finite volume package by NETL (Benyahia et al., 2012). The MFIX two-fluid model (TFM) was used to simulate the hydrodynamics and heat transfer in gas-particle systems. For large-scale simulations the TFM can become computationally intractable. To reduce computation time we employ LES-style sub-grid models (Smagorinsky, 1963) for hydrodynamics (Sarkar et al., 2013) and heat transfer (Lane et al., 2016). The hydrodynamic sub-grid model includes closures for the interphase drag (Igci) and the effective cylinder-suspension drag (Sarkar). Briefly, the Igci interphase drag model is based on the traditional Wen-Yu drag model (Wen and Yu, 1966), incorporating additional terms to compensate for the coarse grid effects. The Sarkar cylinder-suspension drag model replaces the cylinder geometry with an effective porous media (to compensate for the cylinders' volume) and calculates the resulting drag through new source terms. Complete details of the development and implementation of these models can be found in Igci and Sundaresan (2011), Igci et al. (2008), and Sarkar et al. (2013). Verification and validation studies of the models have also been published (Sarkar et al., 2014; Igci and Sundaresan, 2011). The Lane cylinder-suspension heat transfer model (Lane et al., 2014) was developed on the foundation of Sarkar's drag model. The cylinder-suspension heat transfer is approximated with phase-specific heat generation terms. These source terms take the common form of a Nusselt correlation:

$$\overline{Nu}_{cs} = 0.354\,\bar{\phi}_s^{0.125}\left[1 + 2.94\left(\frac{D_c}{a_c}\right)^{1.76}\right]\left(\frac{|\widetilde{\mathbf{v}}_s|}{v_t}\right)^{0.341}\overline{Pe}_{cs}^{0.353}, \tag{1}$$

where $\overline{Nu}_{cs} = \overline{h}_{cs}L^*/k_s$ is the filtered suspension-cylinder Nusselt correlation, $\overline{h}_{cs}$ is the filtered suspension-cylinder heat transfer coefficient, $L^* = v_t^2/g$ is the characteristic length, v_t is the terminal velocity of the solid particles, g is acceleration due to gravity, k_s is the solids conductivity, $\bar{\phi}_s$ is the filtered solids-fraction, D_c/a_c is the ratio of cylinder diameter and spacing, $|\widetilde{\mathbf{v}}_s|$ is the filtered solids velocity, $\overline{Pe}_{cs} = \rho_s C_{p,s} v_t L^*/k_s$ is the filtered Peclet number, rho_s is the solids density, and $C_{p,s}$ is the solids specific heat capacity. This model is used as the basis for the VVUQ studies presented in this work.

Unless otherwise noted, the high-resolution "control" simulations for the verification and validation comparison were calculated using the MFIX default governing equation forms for continuity, momentum, energy, and species transfer (Syamlal and Rogers, 1993). Drag and heat transfer were calculated using the Wen and Yu (1966) and Gunn (1978) models, respectively. The coarse grid simulations used modified governing equations with new constitutive relations for hydrodynamics (Sarkar et al., 2013) and teat transfer (Lane et al., 2016).

3. Verification

To verify the numerical integrity of the new sub-grid model (Syamlal and Rogers, 1993), we considered two small-scale test cases, comparing the transient and steady-state behaviors. Highly-resolved simulations are used as the "control" simulations, while coarse-grid simulations are used to demonstrate the necessity and significance of the sub-grid model. These domains are described in the following sections.

3.1. Case 1: Simple cooling

The first verification case consists of a square periodic domain measuring 3 cm × 3 cm. Cylinders measuring 1 cm in diameter are spaced 1.5 cm apart within the domain (Fig. 1). A mixture of 70% gas and 30% solids occupies the empty region in the system, initialized at 30 °C. The cylinder walls are held at a constant temperature of 20 °C. A pressure gradient Δp_g is imposed along the y-direction, opposing gravity, to drive the flow. This gradient is adjusted to achieve a mean flow velocity of 0.5 m/s upwards. The system is simulated for 10 s, allowing it to reach 90% of thermal steady-state. Material properties are reported in Table 1.

To demonstrate the effects of the grid-dependence and sub-grid models, we consider three configurations (where Δ/d_p is the ratio of grid size, Δ to particle diameter, d_p): (a) highly-resolved grid, $\Delta_{\text{grid}}^{\text{high-res.}}/d_p = 2$, where the cylinder geometry and transport phenomena are fully resolved, (b) coarse-grid, $\Delta_{\text{grid}}^{\text{coarse}}/d_p = 8$, where