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Study of the effect of reactor scale on fluidization hydrodynamics using fine-grid CFD simulations based on the two-fluid model

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ABSTRACT

Reliable scale-up of fluidized beds is essential to ensure that analysis and performance optimization at lab-scale can be applied to commercial scales. However, scaling fluidized beds for dynamic similarity continues to be challenging because flow hydrodynamics at lab-scale are largely influenced by bed geometry making extrapolation of conclusions to large-scales infeasible. Therefore, this study is focused on analyzing the effect of bed geometry on the fluidization hydrodynamics using large-scale CFD simulations. The two fluid model (TFM) is employed to describe the solids motion efficiently and simulations are conducted for fluidization of 1150 μm LLDPE and 500 μm glass beads in beds of different sizes (diameter $D = 15$–70 cm and initial bed height $H_0 = 10$–75 cm). The hydrodynamics are subsequently investigated qualitatively using time-resolved visualizations, bubble centroid and solids velocity maps as well as quantitatively using detailed bubble statistics and solids circulation metrics. It is shown that as the bed diameter is increased, average bubble sizes decrease although similar-sized bubbles rise faster because of lower wall resistance, both factors contributing to faster solids circulation. On the other hand, fluidization hydrodynamics in 50 cm diameter bed are relatively insensitive to the choice of H_0 and similarities in solids circulation patterns are observed in shallow beds as well as in the lower regions of deep beds. Finally, it is shown that the size and spatial-distribution of bubbles is crucial for maintaining dynamic similarity of bubbling beds. Specifically, the bed dimensions (D, H_0) must ensure that (a) bubbles are typically much smaller than the bed diameter and (b) solids circulation patterns are similar across scales of interest. Overall, insights from this study can be used for describing the gas distribution and solids motion more accurately for better design of commercial beds.

1. Introduction

Fluidized beds are commonly used in chemical and petroleum industries due to high heat and mass transfer rates resulting from large gas-solids contacting [1]. However, commercial-scale design and performance optimization of fluidized beds continue to be challenging because of technical limitations of diagnostic techniques in harsh conditions (high pressure and temperature) these beds often operate in. Thus, with the development of numerically efficient solvers and advent of high performance computing (HPC) clusters, computational fluid dynamics (CFD) is expected to play an important role in commercial-scale applications by providing valuable insights into the fluidization hydrodynamics.

To better understand the fundamentals of fluidization i.e. gas (bubble) and solids (dense-phase) motion and interaction, a plethora of experiments have been undertaken in the past few decades. Most measurements are restricted to lab-scale setups: either thin rectangular beds for ease of optical accessibility (e.g. [2–4]) or small-scale cylindrical beds because of limitations on the technical ability [5,6] and accuracy of measurement techniques at large-scales [7,8]. Using analytically derived expressions fitted with experimental data, most studies attempt to characterize bubble growth [9–12] and subsequently, the solids motion [13–16], which are extremely useful for developing accurate submodels and validating CFD simulations. However, inferences from these studies cannot be extrapolated to commercial-scale design and operation. This is because in lab-scale beds, bubble sizes are comparable to the bed diameter (in many cases, slugs are observed) and hence, bubble motion is largely influenced by the presence of walls. Specifically, bed walls constrain the flow aiding bubble coalescence and growth which results in increased bubble sizes. This observation has been reported by both Werther [17] using fine quartz sand (average diameter 83 μm) as well as Glicksman and McAndrews [18] in their fluidization experiments of large sand particles (average diameter 1 mm). On the other hand, similar sized bubbles also rise faster in larger beds due to lower wall resistance [19] and higher porosity of the dense phase [17].

Meanwhile, there is also evidence that the effect of scale decreases with increasing bed diameter, suggesting the notion of a critical

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diameter above which results are scalable. By comparing bubble characteristics across differently sized fluidized beds, Werther [17] and Glicksman and McAndrews [18] independently concluded that wall effects become insignificant in beds larger than 50 cm, suggesting that hydrodynamics in a commercial-scale setup can be analyzed using intermediate pilot-scale beds of diameter 50 cm or more. Strictly speaking, this critical diameter depends on the initial bed height as well as the operating conditions (particle properties and superficial gas velocity) [20]. In case of shallow beds, small bubbles develop close to the walls and laterally coalesce towards the center creating circulation cells where net upflow of solid particles is close to the walls and downflow at the center [21,22]. Bubble sizes in these beds are insignificant compared to the bed diameter and hence, bubble dynamics are largely dependent on the operating conditions and distributor design [23]. On the other hand, if the bed is sufficiently deep, coalescence through the bed leads to the formation of large bubbles (and slugs) which interact with the bed walls [11,20]. It follows that scalability of bubbling fluidized bed results depend on typical bubble sizes in relation to the bed diameter, with Glicksman and McAndrews [18] suggesting that bubbles as small as 20% of the bed diameter experience wall effects.

Fluidization hydrodynamics can be largely characterized by bubbles rising through the bed because bubble dynamics reveal insights into both the gas distribution as well as the solids motion in the bed [7,15]. Thus, early theories were focused on predicting bubble characteristics [10,12,20] and subsequently, explaining bed hydrodynamics by modeling mass and momentum exchange between the bubble and emulsion phases [1]. While these two-phase models are computationally tractable, assumptions regarding bubble properties and gas-flow distribution limit their general applicability. On the other hand, fine-grid CFD simulations are computationally intensive but their robust applicability renders them suitable for predicting the hydrodynamics at large scales. Fluidization simulations typically represent solid particles and describe their motion using (a) Lagrangian framework where individual particles are tracked or (b) Eulerian framework where the solids phase is described as a continuum. While the former models particle-scale interactions rigorously, the Eulerian framework, or two fluid model (TFM), is computationally more efficient and can be used for large-scale simulations. Despite the advantage, however, only few studies have investigated hydrodynamics in large fluidized beds (e.g. [24–27]), most of which are limited to 2D simulations. Thus, there is a strong need for fine-grid 3D simulations to rigorously quantify the effect of scale on fluidization hydrodynamics.

This work is part of a series of studies [27–30] investigating bubbling fluidization of Geldart B particles. Previously, critical sub-models of the TFM were identified and validated by comparing suitable metrics for the gas and solids motion with experimental data. In [28], it was shown that modeling cylindrical beds using cylindrical coordinates is more accurate and efficient as compared to Cartesian coordinates, and challenges associated with the former were addressed including (a) centerline condition to prevent spurious accumulation of solids and (b) constraints on grid resolution for validity of the solids continuum in TFM. In [27], 2D bubble statistics and solids circulation metrics were developed to investigate the role of wall boundary condition in simulations of thin-rectangular fluidized beds, which were later extended to cylindrical beds in [29]. By comparing simulations with experimental measurements spanning a wide range of bed sizes, particle properties and superficial gas velocities, these studies concluded that for dense solid-gas simulations at low superficial gas velocities, the Gidaspow gas-solid drag model [31] is more appropriate and the choice of specularity coefficient ϕ (characterizing particle-wall interactions) must be in the range [0.01,0.3]. Finally in [30], MS3DATA (Multiphase-Flow Statistics Using 3D Detection and Tracking Algorithm) is developed for accurate and efficient characterization of bubbles using temporally and spatially resolved void fraction data from simulations. This methodology is particularly apt for large-scale applications because it overcomes inherent limitations of the conventionally used 2D statistics approach. Specifically, 3D detection enables accurate description of bubble sizes and azimuthal tracking of bubbles, both of which could significantly impact large-scale hydrodynamics. Thus, development of tools and validation of the TFM in [27–30] forms the basis of analysis presented in this study.

The present study is focused on describing the effect of scale (bed diameter D and initial bed height H_0) on the fluidization hydrodynamics, both qualitatively and quantitatively. This analysis will be useful not only for commercial-scale reactor design but also for establishing reduced-order models which can be used in system-level analysis for optimizing conversion efficiency [32–34]. The simulation setup and fluidization metrics are briefly described in Sections 2 and 3 respectively, while detailed description can be found in [29]. Although the simulation setup has been validated previously in terms of bubble dynamics [29], solids velocity predictions are compared with experimental measurements by Laverman et al. [35] in Section 4.1. Validated simulations are subsequently used to analyze the effect of scale on both bubble dynamics and solids circulation in Sections 4.2 and 4.3, respectively. All simulations are performed using MFiX (Multiphase Flow with Interface eXchanges), an open-source code developed at the National Energy Technology Laboratory, USA to describe the hydrodynamics in solid-gas systems.

2. Simulation setup

2.1. Governing equations

For this study, the two-fluid model (TFM) is employed since this approach balances accuracy and computational cost making it suitable for scale-up. The TFM describes both the gas and solid phases as inter-penetrating continua with governing equations similar to single-phase fluid flow. For cold fluidization, the continuity and momentum equations reduce to

$$\frac{\partial}{\partial t}(\varepsilon_k\rho_k) + \nabla\cdot\left(\varepsilon_k\rho_k\vec{V}_k\right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_k\rho_k\vec{V}_k\right) + \nabla\cdot\left(\varepsilon_k\rho_k\vec{V}_k\vec{V}_k\right) = \nabla\cdot\bar{\bar{S}}_k - \varepsilon_k\nabla P_g + \varepsilon_k\rho_k\vec{g} + \left(\delta_{km}\vec{I}_{gm} - \delta_{kg}\vec{I}_{gm}\right) \tag{2}$$

$$\delta_{ki} = \begin{cases} 1 & \text{if } k = i \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

where ε,ρ and $\vec{V}$ are the volume fraction, density and velocity for the gas ($k = g$) and solid ($k = m$) phases. The solids stress tensor $\bar{\bar{S}}_m$ is evaluated using the kinetic theory of granular flow (KTGF) [36] in dilute regions where collisional forces are dominant and Shaeffer's frictional theory [37] in dense pockets of the bed accounting for enduring contact between particles i.e.

$$\bar{\bar{S}}_m = \begin{cases} -P_m^{dense}\bar{\bar{I}} + \bar{\bar{\tau}}_m^{dense} & \text{if } \varepsilon_g \le \varepsilon_g^* \\ -P_m^{dilute}\bar{\bar{I}} + \bar{\bar{\tau}}_m^{dilute} & \text{if } \varepsilon_g > \varepsilon_g^* \end{cases} \tag{4}$$

and the two regimes are blended around ε_g^* using hyperbolic tangent function [38]. In general, the solids stress tensor is dependent on particle properties and local flow conditions including granular temperature which is representative of the kinetic energy associated with the fluctuating component of particle velocity. Thus, the system of equations is closed by solving the conservation of granular temperature Θ_m given by

$$\frac{3}{2}\left(\frac{\partial(\varepsilon_m\rho_m\Theta_m)}{\partial t} + \nabla\cdot\left(\varepsilon_m\rho_m\vec{V}_m\Theta_m\right)\right) = \bar{\bar{S}}_m : \nabla\vec{V}_m + \nabla\cdot\vec{q}_{\Theta_m} - \gamma_{\Theta_m} + \phi_{gm} \tag{5}$$

which considers production $\bar{\bar{S}}_m : \nabla\vec{V}_m$, diffusion $\nabla\cdot\vec{q}_{\Theta_m}$ and dissipation