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Numerical characterization and modeling of particle clustering in wall-bounded vertical risers

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HIGHLIGHTS

- Cluster descent velocities and solid packing match experimental correlations.
- Solid distribution is unaffected by the Archimedes number and follows a lognormal law.
- The standard deviation of volume fraction depends only on the mean concentration.
- The characteristic cluster length scale is limited by the diameter of the reactor.
- 2D simulations grossly over-predict the volume fraction and velocity fluctuations.

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ABSTRACT

This paper aims at investigating the capability of numerical models to accurately capture the physical characteristics of particle clustering in vertical risers. Within the energy sector, particle clustering in vertical risers of circulating fluidized bed reactors are known to play a key role in the multiphase dynamics as well as secondary processes such as catalytic conversion and heat transfer. Recent experiments suggest that particle clustering is most significant in the fully developed flow region of the riser, hence this study focuses on this region. To explore such flows, a high-fidelity large-eddy simulation framework is combined with a Lagrangian particle tracking solver to simulate statistically stationary gravity-driven risers in vertical pipes for a large range of Archimedes numbers. The walls of the reactor are modeled using a conservative immersed boundary scheme integrated with the Lagrangian particle tracking framework. A structure tracking algorithm akin to particle image velocimetry is used to accumulate statistics on individual clusters. Cluster descent velocities display excellent agreement with experimental measurements for the range of flow conditions considered. Predicted volume fraction fluctuations and mean solid concentration within the clusters also match experimental correlations. The probability distribution function of solid concentration and radial distribution function provide insight on the degree of clustering and the characteristic cluster length scale. The degree of particle clustering is found to be independent of the Archimedes number, and models for the volume fraction distribution are discussed. Statistics on the solid concentration and phase velocities for two- and three-dimensional configurations are compared, and the ramifications of simulating risers in two dimensions are discussed.

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1. Introduction

Particle-laden flows in vertical pipes play a crucial role in many industrial processes. Within the energy sector, such flows are used in fluidized bed reactors due to their low pressure drops, uniform temperature distribution, and high efficiency in mixing. Since the 1970s, circulating fluidized bed (CFB) reactors have been used in a range of technical processes, including fluid catalytic cracking (FCC) [1,2], gasification and combustion of coal [3–5], and more recently thermochemical conversion of biomass [6,7]. CFB reactors were developed to improve the performance of traditional fluidized beds by using higher flow rates to move the bed material resulting in a significant increase in the contact efficiency between the phases. This increased kinetic energy within risers of CFB reactors causes the flow to become unsteady with large particle concentration fluctuations. Local regions of densely packed particles, referred to as clusters, develop in the flow and tend to fall at the walls of the riser, while dilute suspensions of particles rise in the central region. Sustained volume fraction and velocity fluctuations

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caused by the clusters result in the production of fluid-phase turbulent kinetic energy, which then exists even in the absence of mean shear [8]. Meanwhile, under specific conditions, clusters have been observed to reduce mixing and interaction of particles with the transport gas [9], and therefore may inhibit reaction rates and heat transfer in industrial units, potentially lowering operating efficiencies significantly. Without the ability to predict and optimize reactor performance, large-scale commercialization of these systems remains severely restricted.

Because the solid phase is opaque and highly unsteady, experimental studies on particle clustering in risers have proven to be an arduous task. Nonetheless, many correlations of cluster characteristics have been derived from experimental data. Noymer and Glicksman [10] compiled numerous measurements of cluster fall velocities from within the literature, observing that although the flow conditions vary significantly, as well as the reactor geometries and particle parameters, the measured velocities were typically close to 1.0 m/s. Previous investigations on risers indicate that clusters tend to fall within 100 μm of the wall [11], placing them within the hydrodynamic boundary layer. Additionally, particles tend to reduce the gas-phase velocity gradients [12], implying that clusters falling near the walls are generally unaffected by the superficial gas velocity. Noymer and Glicksman [10] developed a model to match the observed trends for the measured cluster fall velocities, given by

$$u_{cl} = 0.75\sqrt{\frac{\rho_p}{\rho_f} g d_p}, \tag{1}$$

where ρ_p and ρ_f are the particle and fluid densities, respectively, g is the gravitational acceleration, and d_p is the particle diameter. Note that the cluster velocity u_{cl} is independent of the gas-phase viscosity and mass flow rate. Recent studies by Chew et al. [13–16] used a fiber optic probe and high-speed video camera to characterize clustering of monodisperse and polydisperse particles in a riser of a pilot-scale CFB. It was found that the riser axial position greatly influences the radial profiles of cluster duration and frequency, but has negligible effect on cluster appearance probability. The particle size distribution and particle properties were shown to have comparatively minor effects on cluster characteristics. Two recent studies [17,18] used high-speed video and wavelet decomposition analysis of backscattered optical data to show that clusters were much more prevalent in the fully developed flow region of the riser. It was concluded that a better understanding of particle clustering and their interactions with the gas phase is clearly needed to improve existing models found in the literature.

With increasing computational resources and advancements in numerical methods, many researchers have turned to computational fluid dynamics (CFD) to gain further insight on particle clustering in risers. There exists a spectrum of modeling approaches for simulating coupled fluid-particle flows, each with its own advantages and disadvantages. In recent years, particle-resolved direct numerical simulations (PR-DNS) of three-dimensional gas-solid flows with $\mathcal{O}\left(10^4\right)$ particles have become feasible. A recent review article on PR-DNS development can be found in [19]. To the best of the authors' knowledge, state-of-the-art PR-DNS is currently unable to resolve the necessary length scales required in simulating freely-evolving clusters in risers due to excessive computational cost. However, recent efforts have focused on model development for lower cost simulation techniques. For example, Xu and Subramaniam [20] performed PR-DNS of a turbulent flow past uniform and clustered configurations of fixed particle assemblies using a discrete-time, direct-forcing, immersed boundary method. The fluid-phase turbulence was found to be significantly anisotropic due to the fluid-particle interaction, and the level of turbulent kinetic energy in the fluid phase was always found to be greater in the clustered case compared to the uniform particle configuration. Another recent study [21] conducted lattice Boltzmann simulations of a single fixed cluster under a wide range of volume fractions and particle Reynolds numbers. The PR-DNS results revealed that particles arranged in a cluster configuration exhibited considerably lower drag than randomly arranged particles under the same flow conditions, with more significant reduction at lower particle Reynolds numbers.

In order to investigate realistic riser configurations in a tractable manner, Eulerian–Eulerian (EE) and Eulerian–Lagrangian (EL) methods have been used in numerous studies within the literature with various levels of success. EE representations solve the gas phase and solid particles on a common Eulerian grid, greatly reducing the computational cost as individual particles do not need to be tracked. In the limit where the flow is highly collisional and assumed to be nearly at equilibrium, the particle density function is close to Maxwellian and a Chapman–Enskog expansion can be used to derive a two-fluid model (TFM) using ensemble or volume averaging [22–24]. TFM has been used in a large number of studies to simulate two-dimensional (e.g., [25–31]) and three-dimensional (e.g., [32–35]) risers. Most of this work extracts mean profiles of the hydrodynamic variables, typically the solid volume fraction, pressure drop, and velocity of each phase. Chalermsinsuwan et al. [36] compared particle cluster diameter and concentration in risers using two-dimensional TFM. The calculated values were comparable to empirical correlations. Agrawal et al. [32] demonstrated that global statistics were strongly dependent on the mesh size but became mesh-independent when mesh size was of the order of a few particle diameters. Furthermore, it was shown that clusters are not properly captured unless sufficient resolution is applied. Ozel et al. [33] employed TFM in a recent work at various resolutions to obtain mesh-independent results in periodic CFB risers. It was shown that various sub-grid terms have to be modeled in order to account for the unresolved clusters.

EL strategies provide an alternative framework that typically relies on simpler closures compared to EE, where individual particle trajectories are solved using Newton's laws of motion, and models are required for interphase exchange and particle collisions. Particle clustering in two-dimensional risers using the EL method can be found in a large number of studies from previous years (e.g., [37–42]). In these studies, large-eddy simulation (LES) is often used to solve the gas-phase turbulence, and particle collisions are typically modeled stochastically by means of the direct simulation Monte Carlo (DSMC) method. Liu and Lu [42] used a DSMC-EL approach to study cluster dynamics in a two-dimensional riser. A cluster identification method was used to obtain the solid concentration and velocities of individual clusters. In order to compare their results with experimental data, the computed two-dimensional voidage used in the drag calculation was modeled as three-dimensional using the correction described in [43]. Mean cluster descent velocities as a function of mean solid concentration showed reasonable agreement with experimental correlations. The mean solid concentration of near wall clusters was shown to increase with the increase of cross-sectional averaged solid concentration. The simulated results, however, consistently under-predicted the experimental findings. In a response to this study by Liu and Lu [42], Berrouk and Wu [44] discussed the severe shortcomings of the phase coupling scheme used in the context of two-dimensional EL methods. It was shown that schemes to correct the two-dimensional void fraction under-predict the momentum source term, which results in a much lower prediction of the pressure drop and erroneous prediction of the minimum fluidization velocity. It was concluded that since the pressure gradient force plays a crucial role in the two-phase dynamics, two-dimensional EL methods may systematically provide an inaccurate