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Effect of a cluster on gas–solid drag from lattice Boltzmann simulations

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HIGHLIGHTS

- LB simulations of gas–solid flow with a single cluster were conducted.
- The study quantifies reduction in the gas–solid drag due to formation of a cluster.
- Effects of cluster properties on the drag have also been investigated.
- Significant drag reduction was found between a cluster voidage of maximum and 0.7.
- At a fixed cluster voidage, a minimum drag force occurred around 0.96 overall voidage.

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ABSTRACT

Fast fluidization of fine particles leads to formation of particle clusters, which significantly affects the drag force between the phases. Existing gas–solid drag models, both empirical and theoretical, do not account for the effect of the clusters on the drag force, and as a result, the computational studies using them are unable to capture the inherent heterogeneity of fast fluidization beds. The limitation of the current drag models is generally attributed to poor understanding of the effect of the clusters. In this study, the effect of a single cluster on the drag force has been investigated by conducting lattice Boltzmann simulations of gas–particle flow under a wide range of the overall voidage and particle Reynolds numbers. It was observed that simulations with the particles in a cluster configuration gave considerably lower drag than those with particles in a random arrangement. Furthermore, for the cluster voidage between maximum to 0.7, a significant drag reduction was observed when the inter-particle distances within a cluster was decreased. The simulations with a constant cluster voidage of 0.7 showed that the drag force decreased on decreasing the overall voidage from the maximum voidage to approximately 0.96; however any further decrease in the overall voidage caused a steep increase in the drag force. The results of this study are important in quantifying the drag reduction due to the formation of clusters.

1. Introduction

Gas–solid flow under fast fluidization conditions underpins some important chemical processes such as fluid catalytic cracking and circulating fluidized bed combustion. Computational fluid dynamics (CFD) based gas–solid flow models have been extensively applied to investigate the hydrodynamics of fast fluidized beds and carry out possible design improvements (Sundaresan, 2000; Ranade, 2001). All CFD models must include mass and momentum conservations for both gas and solid phases along with a model for inter-phase drag, which strongly affects the simulation results. Most commonly used empirical gas–solid drag models reasonably predict the drag force for voidage at two extremes i.e. maximum and minimum fluidizing voidage. However none of these models account for the effect of formation of particle aggregates, the so called clusters, which occurs at intermediate voidage. This work focuses on quantifying the effect of clusters on the gas–solid drag. Conventional drag models are either derived from pressure drop data under packed bed conditions e.g. the Ergun model (Ergun, 1952), or from single particle settling experiments e.g. the Wen–Yu model (Wen and Yu, 1966), or a combination of these e.g. the Gidaspow drag model (Gidaspow, 1994). To account for the effect of clusters, the conventional drag models have been modified using multi-scale approaches such as sub-grid scale (Andrews et al., 2005) and energy minimization approaches (Li and Kawauk, 1994). Despite

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such modifications, the CFD models shows little qualitative agreement with experimental data (Benyahia, 2009; Shah et al., 2011). Accurate prediction of dilute gas–solid flows therefore needs improved drag models, which require better understanding of the effect of clusters. In this study, the effect of a single cluster on gas–solid drag is computationally investigated.

Available multiphase experimental techniques such as the magnetic resonance imaging, computer tomography and radioactive particle tracking are ineffective in capturing data at the spatio-temporal scales required to analyze the gas-solid interactions at cluster level. On the other hand, direct numerical simulations (DNS) of gas–particle flow can provide this information at a much smaller time and length scales (Yang et al., 2000; Hill et al. 2001a, b; Biggs et al., 2003; Van der Hoef et al., 2005; Beetstra et al., 2007; Yin and Sundaresan, 2009; Garg et al., 2011; Tenneti et al., 2011). Two different numerical approaches, namely lattice Boltzmann method (LBM) and immersed boundary method (IBM) have been previously used to simulate gas-solid flow in order to study the interactions between two phases. Ladd (1994a, b) developed an effective LB method for simulating particle–fluid suspension and also LB code "SUSP3D", which has been used (Hill et al., 2001a, b; Van der Hoef et al., 2005; Yin and Sundaresan, 2009). In the LBM, the flow domain is represented by a number of lattices and the fluid flow is calculated by updating velocity distribution at each lattice by using Boltzmann's velocity distribution function. The flow of particles is resolved by applying Newton's force balance equation. The force interactions between the fluid and particle are then calculated from the velocity distributions at the boundary nodes and velocity of particles. The IBM has been used by Uhlmann (2005); Garg et al. (2011) and Tenneti et al. (2011) to study the drag between the gas and solid phases. In the IBM, the fluid is represented in an Eulerian framework, whereas the particles are represented in a Lagrangian framework. The Eulerian variables are defined on a Cartesian mesh, and the Lagrangian variables are defined on a curvilinear mesh that moves freely through the cartesian mesh without being constrained to adapt to it in any way at all. The fluid–solid interactions are accounted via a smoothed approximation to the Dirac delta function (Peskin, 2002).

Hill et al. (2001a, b) used the LBM to study the drag force on spheres, and provided first numerical observations which showed that the gas-solid drag over a range of solid volume fractions was different from that calculated using the conventional drag models. However, their simulations were limited only to low particle Reynolds numbers and mono-dispersed randomly or regularly arranged particles. Van der Hoef et al. (2005) conducted LB simulations of fluid flowing past mono- and bi-disperse random arrays of spheres to measure the drag force on the spheres for a range of volume fractions and particle Reynolds number. They proposed a correlation for the drag force applicable to both mono- and poly-disperse systems. Beetstra et al. (2006) further extended the LBM study by simulating particles arranged in cluster configurations. The numerically calculated drag coefficients were compared with the experimental data of drag coefficients for irregularly shaped particles reported by Tran-Cong et al. (2004). Beetstra et al. (2006) predicted a strong effect of inter-particle distance on the gas–solid drag force. However, this study was limited only up to 32 particles, and did not include the effect of particle Reynolds number on the drag force. Most of the simulations carried out by Beetstra et al. (Van der Hoef et al., 2005; Beetstra et al., 2006) used a constant particle resolution in all simulations, including those with higher Reynolds number. At higher Reynolds numbers their resolution was not sufficient to resolve the boundary layer thickness around the particle resulting into erroneous drag values. This has been critically highlighted by Tenneti et al. (2011). Tenneti et al. (2011) also strongly suggested requirement of high resolution LBM simulations. Yin and Sundaresan (2009) used the LBM to simulate flow with mono- and bi-dispersed particles, and gave a drag correlation for Stokes flow in fixed particle configuration. Recently, Zhang et al. (2011) simulated a 2D periodic array of clusters using the LBM to investigate the effect of cluster on the drag coefficient. They found close agreement between the simulated drag values and those calculated from the energy minimization approach.

While there are several detailed gas-solid flow simulations, the effect of clusters on the gas-solid drag is still poorly understood. The present study aims to quantify the effect of a single cluster on gas-solid drag by conducting high resolution 3D LB simulations. The simulated flow domain was a cube with periodic boundary conditions, where solid particles were positioned in either random or a cluster configurations. In the cluster configuration, most of particles (up to 1000) were positioned close to each other forming a single cluster with few particles located around the cluster forming a dilute phase. Simulations were carried out with different cluster configurations by varying both overall voidage of the flow domain and voidage of cluster. Furthermore, the flow conditions in these simulations were also varied to cover a wide range of particle Reynolds number from 21 to 210. Simulations results were the drag forces for both the flow domain with random and cluster configurations, which were compared and analyzed in order to quantify the effect of a cluster.

2. Lattice Boltzmann method

This section is intended to give a brief introduction to the LBM for modeling of multiphase flows. For a more detail understanding of the LBM for multiphase flows, readers are referred to Ladd (1994a, b) and Van der Hoef et al. (2005). LBM is a direct numerical simulation technique which resolves the flow of fluid by solving the Boltzmann equation of velocity distributions. The movement of particles is calculated by solving Newton's force balance equation for each particle. The momentum exchange between the fluid and particles is resolved by applying the bounce back rules at boundary nodes.

2.1. Flow of fluid

Flow domain is as number of discrete lattice nodes in x, y and z directions. Each node represents a fluid element with its velocity distributed in 19 directions (D3Q19). At each fluid element, the velocity distribution is updated by the Boltzmann equation:

$$f_a(x+e_a,\ t+\Delta t) = f_a(x,t) - \frac{[f_a(x,t) - f_a^{eq}(x,t)]}{\tau/\Delta t} \quad (1)$$

where f_a is velocity distribution at any lattice node x, e_a is the direction vectors, τ is a relaxation time, and Δt is the time for the fluid elements to travel from node to node. The velocity distribution function, $f_a(x,t)$, describes number of gas elements at lattice node x and time t with a velocity in e_a direction. The magnitudes of velocity direction vectors e_0, e_{1-6} and e_{7-19} are 0 (particle at rest), 1 and $\sqrt{2}$ respectively.

Eq. (1) has two parts, where (i) $f_a(x+e_a,\ t+\Delta t) = f_a(x, t+\Delta t)$ represents streaming; and (ii) $f_a(x,\ t+\Delta t) = f_a(x,t) - [f_a(x,t) - f_a^{eq}(x,t)]/(\tau/\Delta t)$ represents collision steps. Collision is represented by a relaxation towards equilibrium, and the relaxation time controls the kinematic viscosity of the LB fluid (Bhatnagar et al., 1954).

The most common approach to model the relaxation is the Bhatnagar–Gross–Krook (BGK) approach (Bhatnagar et al., 1954); where the relaxation time, τ is governed by the kinematic viscosity of the fluid, with length being represented in terms of lattice units