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Structure-dependent drag in gas–solid flows studied with direct numerical simulation

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HIGHLIGHTS

- Heterogeneity should be included explicitly in drag correlation.
- Linear dependence of drag on Re is validated for fixed heterogeneity in $5 < \mathrm{Re} < 30$.
- The traditional drag law is inadequate for dynamic gas–solid suspensions.

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ABSTRACT

Quantification of drag F is critical to the simulation of gas–solid flows in both discrete particle models and two-fluid models. It is commonly accepted that for homogeneous flow the drag is a function of solid volume fraction ϕ and particle Reynolds number Re_p (based on the mean slip velocity and particle radius). However, its adequacy for heterogeneous flows encountered more frequently is in debate yet. In this work, we reveal the strong structural dependence of the drag in both a simple case of two particles and a typical case with stepwise heterogeneity, demonstrating the necessity for a structure-dependent drag description. To quantify such dependence, flow past idealized static suspensions with linear heterogeneity is studied first, which confirms a general form $F(Re_p,\phi,|\nabla\phi|,\theta)$ suggested previously, where θ is the angle between the gradient $\nabla\phi$ and the mean slip velocity. In the studied range of $5 < Re_p < 30$, F depends linearly on Re_p for a given static particle configuration. However, the concrete expressions are yet to be found. Then for dynamic gas–solid suspension, large-scale simulations enabled by supercomputing systems reveal a much more complicated dependence: on one hand, the drag coefficients on individual particles scatter even in the absence of distinct heterogeneity; and on the other hand, with the presence of distinct heterogeneity, the drag predicted by Wen and Yu (1966) deviates significantly from the simulation value in both direction and magnitude. A purely bottom-up statistical approach to establish a drag correlation in this case seems difficult and a theoretical elucidation is needed.

1. Introduction

Gas–solid flows are characterized by strong multi-scale heterogeneity in both time and space (Li and Kwauk, 2001), such as in fluid catalytic cracking (FCC) of heavy oil and coal gasification (Avidan et al., 2011), which proposes great challenges to the quantification and prediction of their hydrodynamic behavior through theoretical treatment, physical experiment, or computer simulation.

In terms of computer simulation, most researches so far have employed the so-called two-fluid models (TFM, Anderson and Jackson, 1967) and discrete particle models (DPM, Tsuji et al., 1993). Both models assume that at scales much larger than that of the solid particles, the averaged fluid phase is continuous, which validates an Eulerian description based on the volume-averaged Navier–Stokes equations. For the solid phase, the former adopts an Eulerian approach similar to that of the gas phase while the latter employs a Lagrangian approach to track the motion of each solid particle individually. For both models, the interphase momentum transfer term distinguishes them from single phase Navier–Stokes equations and is significantly affected by the heterogeneity of gas–solid flows (Li and Kwauk, 2001). The drag caused by the relative motion between the two phases is the predominant component in

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this interaction. Though it has attracted decades of extensive research, a reliable quantification of the heterogeneity effect on the drag is yet to be obtained. Ten years ago a structure-dependent drag model was proposed (Yang et al., 2003), which has improved significantly the accuracy of TFM. It is based on the so-called Energy Minimization Multi-Scale (EMMS) model (Li, 1987; Li et al., 1988; Li and Kwauk, 1994), which describes the heterogeneity in concurrent-up gas–solid flow in terms of decomposed dense and dilute phases. In recent years, more and more studies (Beetstra et al., 2006; Ten Cate and Sundaresan, 2006; Zhang et al., 2011) have demonstrated the necessity of this approach, and other models were proposed to consider the effect of unresolved structures on the drag, e.g., the filtered two-fluid models based on fine-grid simulation (Igci et al., 2008; Parmentier et al., 2012).

However, these studies so far are mainly focused on scales above the characteristic length of the heterogeneous structures, such as the bubble or cluster diameter. Such characteristic scale is usually termed as meso-scale (Li and Kwauk, 2001). In fact, the EMMS model is valid both at and above the meso-scale (Zhang et al., 2005). Whether fine-grid simulations below the meso-scale can finally reproduce the macroscale flow behavior without introducing a modified drag correlation, and, if not, whether new parameters, such as the gradients of the flow variables (Marchioro et al., 2000; Ten Cate and Sundaresan, 2006), should be introduced into the drag correlation to account for the effect of the heterogeneity remain as open questions.

In fact, Li et al. have shown in the development of the EMMS model that the magnitudes of the drag coefficients in the dense and dilute phases and on their interface can be different in orders (Li et al., 1993), for which we have discussed previously a simple case, that is, the stepwise heterogeneity (Ge, 1998), to elaborate such drag distribution. Inspired by these studies, Xu et al. (2007) proposed a computational scheme to account for the effect of heterogeneity on the drag distribution in a DPM element by assuming linear variation of ϕ and introducing its gradient as a new parameter. Nevertheless, we are still short of systematic study about the effect of heterogeneity on the drag with fully-resolved simulation. In recent years, the dramatic development of super-computing, especially the combination of many-core parallelization and scalable flow solvers has brought about new possibilities (Wang et al., 2010; Xiong et al., 2010, 2012), that is, direct numerical simulation (DNS), where the Navier–Stokes equations are solved directly with the no-slip boundary conditions enforced on particles' surfaces and the drag is obtained by integrating the stress on these surfaces. It is believed to give the most fundamental and reliable numerical description of the drag. The lattice Boltzmann method (LBM) (McNamara and Zanetti, 1988) is chosen to solve the fluid phase due to its high efficiency, intrinsic parallelism and inherent adaptability to complex geometries. Hill et al. (2001a, 2001b) applied the method to study flow past ordered and random arrays of particles for a wide range of particle Reynolds number Re_p and solid volume fraction ϕ, and finally expressed the drag as a function of these two variables. A series of publications on the drag have followed with different focuses, varying from low (Van der Hoef et al., 2005; Yin and Sundaresan, 2009) to high Reynolds numbers (Beetstra et al., 2007; Holloway et al., 2010), from mono- to bi-disperse particles (Van der Hoef et al., 2005; Beetstra et al., 2007; Holloway et al., 2010; Yin and Sundaresan, 2009), and with or without (Tenneti et al., 2010, 2011) consideration of granular temperature. In all these works, however, all the particles were uniformly distributed throughout the domain during the simulations, so all the systems were supposed to be homogenous.

In this study, to reach some definite conclusions about the effect of heterogeneity on the drag, the study will be limited to some specific cases. We will first study two very elementary structures, that is, a pair of isolated particles and a typical structure with stepwise heterogeneity. Then to get a more quantitative understanding of the effect, we work on a relatively easy but idealized case where ϕ displays a linear heterogeneity which can be clearly quantified by its gradient $\nabla\phi$. To be more specific, we confine the simulations to only two typical ϕ values in the range $5 < Re_p < 30$ (Re_p is based on particle radius), where, as we know for the homogeneous structure, the drag depends linearly on Re_p at constant ϕ (Hill et al., 2001a, 2001b). Quite a few engineering systems fall into this range, such as circulating fluidized bed coal combustion (Zhu et al., 1995). Although the particles are kept static in this case, it is still relevant to dynamical gas–solid flows since the typical Stokes number St here may reach up to $O(10^4)$. Larger particle inertia means that the response time of the particle dynamics to the flow disturbance is much longer than the characteristic time in fluid flow, so that the hydrodynamics in a typical gas–solid suspension resembles that in a corresponding fixed bed, which is the prerequisite to establish drag models with fixed beds. We finally analyze the drag distribution in a dynamical gas–solid suspension simulated under periodic boundary condition, aiming to get closer to the effect of heterogeneity on the drag in real systems.

2. Numerical method

LBM can be considered as an approach to solve the discretized Boltzmann equation on regular lattices where the fluid is modeled as fictitious particles. At each time step, the particle distribution function f_i in one of the discretized directions, i (typically the orthogonal and diagonal directions in the Cartesian coordinates), is solved as the primary variable through the standard evolution equation (McNamara and Zanetti, 1988)

$$f_i(\mathbf{x}+\mathbf{e}_i\Delta t, t+\Delta t) = f_i(\mathbf{x}, t) + \frac{1}{\tau}(f_i^{\mathrm{eq}}(\rho, \mathbf{v}) - f_i(\mathbf{x}, t)), \tag{1}$$

where τ is the dimensionless relaxation time. Also in Eq. (1), ρ and $\mathbf{v}$ are the density and velocity of the fluid, respectively, which both are functions of time and space. f_i^{eq} is the equilibrium distribution function defined as (Qian et al., 1992)

$$f_i^{\mathrm{eq}}(\rho, \mathbf{v}) = \omega_i\rho\left(1 + \frac{\mathbf{e}_i\cdot\mathbf{v}}{C_s^2} + \frac{1}{2}\frac{(\mathbf{e}_i\cdot\mathbf{v})^2}{C_s^4} - \frac{1}{2}\frac{\mathbf{v}\cdot\mathbf{v}}{C_s^2}\right), \tag{2}$$

where $\mathbf{e}_i$ and ω_i are the unit vector and the lattice weight along direction i, respectively. C_s is the speed of sound which equals $\sqrt{3}/3$ in lattice unit. The dimensionless relaxation time τ is related to the fluid viscosity by the following expression:

$$\nu = \frac{1}{3}(\tau - 0.5)\frac{h^2}{\Delta t} \tag{3}$$

where h and Δt are the space and time steps, respectively.

The standard D3Q19 model with 19 discrete velocities in the three dimensional discrete space (d'Humières et al., 2002) is used here. The computation is split into the propagation step and the collision step. At the propagation step, the particle propagates to its nearest neighbors along each corresponding direction via the distribution function, so the propagation operation involves only its nearest neighbors. Meanwhile, the collision step is considered as a relaxation towards a local equilibrium state that involves the variables associated with only each node itself; therefore the step has purely local operations only. The locality of the evolution brings about significant advantage to LBM in its parallelization.

When LBM is employed to solve gas–solid flows, an extra module has to be incorporated to deal with the fluid–solid coupling. In the work of Ladd (1994a, 1994b), a modified bounce-back rule is adopted to implement the no-slip boundary condition, which results