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A drag force correlation for approximately cubic particles constructed from identical spheres

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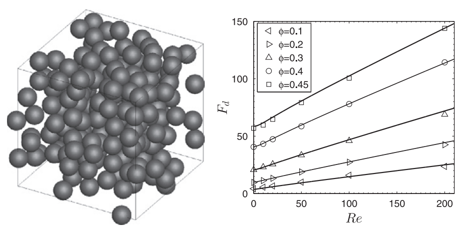
HIGHLIGHTS

- The LBM has been used to develop a drag force correlation for approximate cubes.
- Comparison with correlations for spheres indicates that particle shape is important.
- The new correlation allows an examination of particle shape effects in CFD-DEM models.

GRAPHICAL ABSTRACT



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ABSTRACT

The lattice Boltzmann method has been used to compute the drag force acting on assemblies of approximately cubic particles constructed from eight spheres for a wide range of Reynolds numbers. Based on the simulation data we propose a new drag force correlation for assemblies of approximately cubic particles. We have compared the drag force obtained with that predicted by the correlation proposed by Beetstra et al. (2007), originally proposed for spheres, by considering either the drag acting on individual spheres or the drag acting on an approximately cubic particle composed of eight spheres. The comparisons showed that Beetstra's correlation cannot predict the system well. The correlation proposed in this paper enables Euler–Euler and Euler–Lagrangian simulations of approximately cubic particles, allowing the influence of the solid volume fraction in these models to be assessed.

1. Introduction

Gas–solid systems are of significant industrial importance and are the basis of various reactor concepts, e.g. gas-fluidized and packed beds or rotary kilns. However, with regard to numerical modeling of these systems, very little is known about the force exerted on the individual particles when a fluid flows through an assembly of particles, i.e. the drag force. A good understanding of particle–fluid interactions is essential to predict more accurately the dynamics of these systems. In previous studies, it was found that the pattern formation in gas fluidized beds was significantly affected by the momentum exchange between the gas phase and the solid phase (Li and Kuipers, 2003). A theoretical solution for the drag acting on an isolated sphere in unbounded flow was derived only for the zero Reynolds number limit. Hinch (1977) calculated the drag force for random assemblies of spheres in dilute suspensions by taking into account the presence of neighboring particles. Kim and Russel (1985) extended the work of Hinch (1977), and proposed a drag force correlation for volume fractions up to 0.5, but only the first few terms ($O(\phi^2)$) can be evaluated analytically. For large volume fractions, the drag force can be estimated from the Carman equation (1937). However, the practical value of these theories is rather limited since they are only valid for very low Reynolds numbers. The interaction of particles with a fluid can also be modeled using Stokesian

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Dynamics (Brady and Bossis, 1988). However, this method is also restricted to low Reynolds numbers. For this reason, empirical correlations obtained from pressure drop measurement or terminal velocities measurement of sedimenting particles for higher Reynolds numbers and volume fractions are commonly used in engineering practice, i.e. correlations of Ergun (1952) and Wen and Yu (1966). In recent years, drag laws generated from direct numerical simulations have become available. Koch (Koch and Sangani, 1999; Hill et al., 2001a,b) was the first to develop a drag force correlation based on lattice Boltzmann simulations. Van der Hoef and Beetstra (van der Hoef et al., 2005; Beetstra et al., 2007) extended the work of Hill et al. (2001a,b), establishing new drag force correlations for mono- and bi-disperse arrays of spheres. In these simulations the flow field around a random array of spheres was computed using the lattice Boltzmann method with a lattice spacing that was sufficiently small to allow the detailed flow around the spheres to be modeled. Coupled computational fluid dynamics-discrete element method (CFD-DEM) simulations (Bokkers et al., 2004) performed using the drag model proposed by Hill et al. (2001b) showed better agreement with experimental measurements than those performed using the traditional Ergun and Wen and Yu correlations.

In most practical applications of gas-fluidized beds, the particles are not spherical and the drag force is affected by solid volume fraction and particle orientation. Due to a lack of drag force correlations for assemblies of non-spherical particles, numerical simulations of gas-fluidized beds have largely been restricted to beds containing spherical particles. The effect of particle shape on the drag force has been investigated for isolated particles. For example, Tran-Cong et al. (2004) measured the drag force coefficients for isolated non-spherical particles constructed from several identical spheres. Beetstra et al. (2006) performed LBM simulations of individual non-spherical particles constructed from spheres. Excellent agreement was reported between the LBM data and the experimental results given by Tran-Cong et al. (2004). Hölzer and Sommerfeld (2008), using experimental data and numerical simulations, correlated the drag force acting on single non-spherical particles with particle orientation and Reynolds number. However, these correlations cannot be applied directly to simulate gas-fluidized beds since they do not account for the influence of the solids volume fraction on the drag coefficient. In this paper, we use the lattice Boltzmann method to develop a drag force correlation for an assembly of approximately cubic particles that are constructed from eight identical spheres, a common approach in the DEM. The approximately cubic particles constructed this way are unbreakable and undeformable. The effect of the solid volume fraction and the Reynolds number on the drag force is studied in detail. The new drag force correlation proposed here is suitable for Euler–Euler and Euler–Lagrangian simulations of gas-fluidized beds composed of approximately cubic particles.

2. Drag force correlations for mono-disperse spheres

The total average fluid–particle interaction force acting on each particle within a volume V is usually expressed as

$$\vec{F}_{tot} = \frac{-\phi V}{N} \triangledown P + \vec{F}'_d \tag{1}$$

where $\triangledown P$ is the pressure gradient across the volume, ϕ is the solid volume fraction, N is the number of particles in the volume, $\vec{F}'_d$ is the average drag force due to fluid-solid friction at the surface of the sphere. The total average force $\vec{F}_{tot}$ is determined as $(1/N)\sum_N \vec{F}'_{tot}$, where $\vec{F}'_{tot}$ is the total force acting on each particle in the computational domain calculated by Eq. (24). From a force balance over volume V, we obtain $-V \triangledown P = NF^{\rightarrow}{}_{tot}$. Substituting $-V \triangledown P = N\vec{F}_{tot}$ into Eq. (1) gives an expression to calculate $\vec{F}'_d$, with $\vec{F}'_d = (1-\phi)\vec{F}_{tot}$. In this paper, we define F_d ($F_d = \vec{F}'_d / 3\pi\mu\vec{U} d_p$, $\vec{U}$ is the superficial velocity, d_p is the diameter of the particle, μ is the dynamic viscosity) as the normalized drag force, which is the common choice in chemical engineering (Di Felice, 1995).

Ergun (1952) derived a correlation from pressure drop measurements for a packed bed

$$F_d = \frac{150}{18}\frac{\phi}{(1-\phi)^2} + 1.75\frac{Re}{18(1-\phi)^2} \tag{2}$$

It should be noted that Ergun carried out the experiment with a small range of porosities (0.43–0.54), therefore, the correlation is typically valid for low porosity systems. Wen and Yu (1966) proposed a different type of correlation obtained from measurement of terminal velocity of the sedimenting particles

$$F_d = \begin{cases} \left(1+0.15\,\mathrm{Re}^{0.687}\right)(1-\phi)^{-3.65} & \text{for Re} < 1000 \\ \dfrac{0.44\,\mathrm{Re}}{24}(1-\phi)^{-3.65} & \text{for Re} > 1000 \end{cases} \tag{3}$$

Currently, these two drag force correlations are widely used in CFD simulations. However, it is still unclear whether the correlations can be used for all solid volume fractions and Reynolds numbers. With the development of computing power, direct numerical simulations (DNS) can be employed to derive the drag force for random assemblies of spheres for a wide range of solid volume fractions and Reynolds numbers, one such approach is the lattice Boltzmann method (LBM). DNS methods give high resolution at the surface of the particles, and the flow around particles can be modeled in detail. Hill et al. (2001a,b) proposed the drag force correlation for random assemblies of spheres using LBM simulations

$$F_d = F_0 + F_3\,\mathrm{Re} \tag{4}$$

with

$$F_0 = \begin{cases} \dfrac{(1-\phi)(1+3/\sqrt{2}\phi^{1/2} + 135/64\phi\ln\phi + 16.14\phi)}{1+0.681\phi - 8.48\phi^2 + 8.16\phi^3} & \text{for } \phi < 0.4 \\ 10\dfrac{\phi}{1-\phi^2} & \text{for } \phi > 0.4 \end{cases} \tag{5}$$

and $F_3 = 0.03365(1-\phi) + 0.106\phi(1-\phi) + (0.0116/(1-\phi)^4)$. Beetstra et al. (2007) modified the Ergun equation in order to account for the effect of moderate fluid inertia on the particles. They proposed the following correlation for the drag force:

$$F_d(\phi,\mathrm{Re}) = 10\frac{\phi}{(1-\phi)^2} + (1-\phi)^2(1+1.5\sqrt{\phi}) + \frac{0.413\,\mathrm{Re}}{24(1-\phi)^2}\left[\frac{(1-\phi)^{-1} + 3\phi(1-\phi) + 8.4\,\mathrm{Re}^{-0.343}}{1+10^{3\phi}\,\mathrm{Re}^{-(1+4\phi)/2}}\right] \tag{6}$$

3. Previous studies of non-spherical particles

3.1. Shape factors for non-spherical particle

So far, nearly all simulations for gas–solid flows are restricted to perfect spheres, since it is very simple to implement (Müller et al., 2008, 2009). However, in most engineering applications the particles are non-spherical, which make them more complicated to analyse. In order to describe the deviation from spherical shape,