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Effect of microstructural anisotropy on the fluid–particle drag force and the stability of the uniformly fluidized state

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Lattice-Boltzmann simulations of fluid flow through sheared assemblies of monodisperse spherical particles have been performed. The friction coefficient tensor extracted from these simulations is found to become progressively more anisotropic with increasing Péclet number, $Pe = \dot{\gamma}d^2/D$, where $\dot{\gamma}$ is the shear rate, $d$ is the particle diameter, and $D$ is the particle self-diffusivity. A model is presented for the anisotropic friction coefficient, and the model constants are related to changes in the particle microstructure. Linear stability analysis of the two-fluid model equations including the anisotropic drag force model developed in the present study reveals that the uniformly fluidized state of low Reynolds number suspensions is most unstable to mixed mode disturbances that take the form of vertically travelling waves having both vertical and transverse structures. As the Stokes number increases, the transverse-to-vertical wavenumber ratio decreases towards zero; i.e. the transverse structure becomes progressively less prominent. Fully nonlinear two-fluid model simulations of moderate to high Stokes number suspensions reveal that the anisotropic drag model leads to coarser gas–particle flow structures than the isotropic drag model.

Key words: complex fluids, instability, suspensions

1. Introduction

Fluidized beds where particles are kept in a suspended state by upward flowing fluid are common in chemical process industries. In most of these beds, the Stokes number, $St = m\dot{u}_t/6\pi\mu_ga^2$, is usually much larger than unity. Here, $m$ represents the particle mass, $\dot{u}_t$ is the terminal settling velocity of an isolated particle, $\mu_g$ represents the fluid viscosity, and $a$ is the particle radius. Such beds are often unstable, with homogeneous suspensions giving way to persistent spatial and temporal inhomogeneities in particle volume fraction and the local average velocities of the fluid and particle phases. An inhomogeneous velocity field can be expected to lead to anisotropic microstructure of the particle assembly with the extent of anisotropy increasing with the Péclet number. In this paper, we examine the influence of this anisotropy on the fluid–particle interaction force. When the particle microstructure is anisotropic, the fluid–particle drag must be modelled via an anisotropic friction coefficient tensor; although this has

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have been recognized in soil mechanics for decades (for example, see Renard & Marsily 1997 and the references cited therein), to the best of our knowledge, the potential influence of this anisotropy on the dynamics of fluidized beds has not been studied in the literature. In the present study, we have first performed lattice-Boltzmann simulations of fluid flow through anisotropic assemblies of spherical particles (at low Reynolds numbers) and determined the friction coefficient tensor for various volume fractions and degrees of anisotropy. The anisotropic microstructures were created by shearing assemblies of rigid particles at different shear rates while maintaining them in a thermostat (i.e. fixed granular temperature). The friction coefficient anisotropy is then related to microstructural anisotropy and modelled in terms of Péclet number $Pe$.

We then present an analysis of the linear stability of the state of uniform fluidization to illustrate the influence of an anisotropic friction coefficient. The growth rate of instabilities in gas-fluidized beds of particles is too rapid to permit experimental observation of the initial stages of the formation of inhomogeneous structures. In contrast, the slower growth rates in liquid–solid systems permit observation of different structures in the hierarchy of instabilities. Convective instabilities in liquid-fluidized beds that take the form of one-dimensional vertically travelling waves (Anderson & Jackson 1969; Ham et al. 1990; Nicolas et al. 1996; Duru & Guazzelli 2002) and two-dimensional structures (Duru & Guazzelli 2002) have been reported. Hydrodynamic models for fluidized beds that treat the fluid and particle phases as interpenetrating continua (the so-called two-fluid models) have been analysed by several researchers to probe the emergence of the inhomogeneous structures; in all these studies, the friction coefficient contained in the fluid–particle drag force model is assumed to be isotropic, corresponding to a locally isotropic particle microstructure (for example, see Anderson & Jackson 1969; Batchelor 1988; Ham et al. 1990; Koch 1990; Koch & Sangani 1999; Jackson 2000). These studies revealed that the state of homogeneous fluidization would first give rise to one-dimensional waves with no horizontal structures. These one-dimensional waves undergo subsequent bifurcations leading to the formation of bubble-like voids in dense fluidized beds, and particle clusters in dilute gas–solid systems (Anderson, Sundaresan & Jackson 1995; Glasser, Kevrekidis & Sundaresan 1996, 1997; Glasser, Sundaresan & Kevrekidis 1998; Agrawal et al. 2001). In the present study, we demonstrate that when the anisotropic friction coefficient is taken into consideration the state of uniform fluidization is predicted to be unstable over a much wider parameter space and that in some regions of the parameter space the dominant mode has both vertical and lateral structures. Incorporation of the anisotropic fluid–particle drag model developed in this work in two-dimensional continuum model simulations of moderate- to high-Stokes-number suspensions illustrates that simulations using an anisotropic fluid–particle drag model will predict coarser gas–particle flow structures than simulations that invoke an isotropic drag model.

2. Continuum models for gas–particle flows

In order to place the objective of the work in more concrete terms, we begin with two-fluid model equations that are commonly used to describe the flow of uniformly sized particles and the interstitial (fluidizing) gas, which are given as

\[
\begin{align*}
\frac{\partial (\rho_g (1 - \phi))}{\partial t} + \nabla \cdot (\rho_g (1 - \phi) \mathbf{u}) &= 0, \\
\frac{\partial (\rho_s \phi)}{\partial t} + \nabla \cdot (\rho_s \phi \mathbf{v}) &= 0,
\end{align*}
\]
where $\phi$ is the particle volume fraction; $\rho_s$ and $\rho_g$ are fluid- and particle-phase densities, respectively; $u$ and $v$ are fluid- and particle-phase velocities, respectively; $\sigma_g$ and $\sigma_s$ are fluid- and particle-phase stress tensors, respectively; $f_D$ is the fluid–particle drag force per unit volume of suspension; $g$ is the gravitational acceleration; $T$ is the granular temperature (defined as the r.m.s. of the particle velocity fluctuations); $q$ is the granular energy flux vector; $\Gamma_{\text{slip}}$ is the rate of production of granular energy through slip between particle and fluid phases per unit volume of suspension; $J_{\text{coll}}$ is the rate of dissipation of granular energy due to inelastic collisions per unit volume of suspension; and $J_{\text{vis}}$ is the rate of viscous dissipation of granular energy per unit volume of suspension. Equations (2.1) and (2.2) represent the continuity equations for particle and fluid phases; (2.3) and (2.4) are fluid- and particle-phase momentum balances; and (2.5) is an evolution equation for the granular energy associated with particle velocity fluctuations. In this work a Newtonian closure

$$\sigma_g = p_s \mathbf{I} - \mu_g^* (\nabla u + (\nabla u)^T - \frac{2}{3} (\nabla \cdot u) \mathbf{I}),$$

is adopted for gas-phase stress tensor where $p_g$ is the gas-phase pressure, $\mu_g^*$ is the effective gas-phase viscosity, and $\mathbf{I}$ is the identity tensor. In general $\mu_g^*$ in the continuum model framework will be different from the molecular viscosity due to pseudoturbulent fluctuations in gas velocity arising due to the presence of particles that serve to enhance momentum transport. However, Agrawal et al. (2001) have shown that two-fluid model predictions are insensitive to the gas-phase viscosity that is used. Therefore, we set $\mu_g^*$ to the molecular viscosity. Several authors have derived constitutive models for $\sigma_s$ and $J_{\text{coll}}$ using the kinetic theory of granular flow (for example, see Lun et al. 1984; Gidaspow 1994; Garzo & Dufty 1999). For the purpose of the present study, we employ the model for $\sigma_s$ and $J_{\text{coll}}$ derived by Lun et al. (1984), and use expressions for the role of the interstitial fluid in the granular energy production ($\Gamma_{\text{slip}}$) and dissipation ($J_{\text{vis}}$) described by Koch & Sangani (1999):

$$\sigma_s = \left( p_s - \frac{1 + e_p}{2} \mu_b \nabla \cdot v \right) \mathbf{I} - 2\mu_s \mathbf{S}, \quad \mathbf{S} = \frac{1}{2} \left( \nabla v + \nabla v^T \right) - \frac{1}{3} (\nabla \cdot v) \mathbf{I},$$

$$p_s = \rho_s \phi (1 + 4\eta \phi g_0) T, \quad \mu_b = \frac{256}{96\sqrt{\pi}} \rho_s d \sqrt{T} \phi^2 g_0, \quad \eta = 1 + \frac{e_p}{2},$$

$$\mu_s = \left( \frac{5\rho_s d \sqrt{T}}{96g_0 \eta (2 - \eta)} \right) \left( 1 + \frac{8}{5} \phi \eta g_0 \right) \left( 1 - \frac{8}{5} \phi \eta (3\eta - 2) g_0 \right) + \frac{3}{5} \eta \mu_b \right),$$

$$\Gamma_{\text{slip}} = \frac{81 \phi \mu_g^2 |u - v|^2 \Xi}{g_0 d^3 \rho_s \sqrt{T}},$$
\[ X = \begin{cases} \left( \frac{1 + 3\sqrt{\phi}/2 + (135/64)\phi \ln \phi + 17.14\phi}{1 + 0.681\phi - 8.48\phi^2 + 8.16\phi^3} \right)^2 \left( \frac{1}{1 + 3.5\sqrt{\phi} + 5.9\phi} \right), & \phi < 0.40, \\ \left( \frac{10\phi}{(1 - \phi)^3 + 0.7} \right)^2 \left( \frac{1}{1 + 3.5\sqrt{\phi} + 5.9\phi} \right), & \phi \geq 0.40, \end{cases} \]  

(2.11)

\[ q = -\kappa \nabla T, \]  

(2.12)

\[ \kappa = \frac{75 \rho_s d \sqrt{\pi} T}{48 g_0 \eta (41 - 33\eta)} \left( \left( 1 + \frac{12}{5} \eta \phi g_0 \right) \left( 1 + \frac{12}{5} \eta^2 (4\eta - 3) \phi g_0 \right) \right) + \frac{64}{24\pi} \left( 41 - 33\eta \right) \eta^2 \phi^2 g_0^2, \]  

(2.13)

\[ J_{vis} = \frac{54 \phi \mu_b T}{d^2} R_{diss}, \]  

(2.14)

\[ R_{diss} = 1 + 3\sqrt{\frac{\phi}{2}} + \frac{135}{64} \phi \ln \phi + 11.26 \left( 1 - 5.1\phi + 16.57\phi^2 - 21.77\phi^3 \right) - \phi g_0 \ln \epsilon_m, \]  

(2.15)

\[ J_{coll} = \frac{12}{\pi} \left( 1 - e_p^2 \right) \frac{\rho_s \phi^2}{d} g_0 T^{3/2}, \]  

(2.16)

where \( \rho_s \) is the particle-phase pressure, \( \mu_b \) is the bulk viscosity of the particle phase, \( \mu_s \) is the particle-phase viscosity, \( \mu_g \) is the gas-phase viscosity, \( e_p \) is the coefficient of restitution, \( \kappa \) is the conductivity, \( R_{diss} \) is the coefficient associated with viscous granular energy dissipation, \( \epsilon_m = 0.01 \), and \( g_0 \) is the radial distribution function at contact for which we use the expression of Ma & Ahmadi (1988)

\[ g_0(\phi) = \frac{1 + 2.5\phi + 4.5094\phi^2 + 4.515439\phi^3}{\left( 1 - (\phi/\phi_m)^3 \right)^{0.67821}}, \]  

(2.17)

where \( \phi_m = 0.64356 \). This form of the radial distribution function was used by Koch & Sangani (1999) in their analysis of the stability of the uniformly fluidized state.

The fluid–particle interaction force \( f_D \) is usually written as

\[ f_D = \beta \left( u - v \right), \]  

(2.18)

where the friction coefficient \( \beta \) is assumed to be isotropic; this is reasonable only if the particle microstructure is isotropic. However, the particle microstructure in fluidized beds is not isotropic (see figure 11a–c). Thus, in writing (2.18), it is implicitly assumed that the microstructural anisotropy is unimportant in the drag force model. In fluidization problems, the weight of the particles is largely supported by the fluid–particle drag, and hence even a small change in the fluid–particle drag can have a large influence on the dynamics. When the microstructural anisotropy is important, the drag force model should be modified as

\[ f_D = \hat{\beta} \cdot (u - v) \]  

(2.19)

where \( \hat{\beta} \) is the friction coefficient tensor, whose diagonal elements will simply be \( \beta \) (equation (2.18)) for isotropic systems. In this study, we ask how significant the anisotropy of \( \hat{\beta} \) is and what its consequence on the state of uniform fluidization is.
In the suspension rheology community, a substantial amount of work has been devoted to describing the rheology of concentrated suspensions in terms of particle microstructure (for example, see Brady & Vicic 1995; Brady & Morris 1997; Stickel & Powell 2005). The changes in particle microstructure upon simple shear deformation have been linked to nonlinear response properties like shear thinning, shear thickening, and normal stress differences (for example, see Phung, Brady & Bossis 1996). The extent of deviation of the particle microstructure from an equilibrium state depends on the Péclet number

\[ Pe = \frac{\dot{\gamma} d^2}{D} = \frac{\dot{\gamma} d \phi g_0(\phi)}{\sqrt{T} \sqrt{\pi}}, \]

(2.20)

where the shear rate \( \dot{\gamma} = \sqrt{2(E:E)} \), and the deformation rate tensor \( E = (1/2)(\nabla v + \nabla v^T) \). In (2.20) we have used the expression for the self-diffusivity \( D \) that was derived by Savage & Dai (1993) using the fact that the particles in this study interact through elastic collisions (namely \( \epsilon_p = 1 \)). It should be noted that for sheared systems the shear-induced self-diffusivity is known to be anisotropic (Drazer et al. 2002; Abbas, Climent & Simonin 2009). However, since we only seek a scale for the self-diffusivity, we use the scalar expression for the self-diffusivity described by Savage & Dai (1993) for the sake of simplicity. When the magnitude of shearing is weak compared to diffusion, the Péclet number is small and the particle microstructure resembles that of an equilibrium configuration of spheres; however, as the Péclet number is increased beyond unity substantial anisotropy develops in the particle microstructure. In this study we focus on how shear deformation affects the magnitude and direction of the fluid–particle drag force experienced by an assembly of spherical particles. In fluidized systems, we note that additional mechanisms for the development of anisotropic and inhomogeneous microstructure exist. For example, inelastic collisions between particles have been observed to create highly anisotropic and inhomogeneous clustering phenomena (Goldhirsch & Zanetti 1993); this mechanism for clustering further accentuates the hydrodynamic clustering that occurs naturally in fluidized suspensions (Sundaresan 2003).

In most gas–particle fluidized beds, the Reynolds number based on particle diameter and the fluid–particle slip velocity is \( O(1) \) or smaller; thus, the inertial correction to the fluid–particle drag force is quite small (Beetstra, Van Der Hoef & Kuipers 2007). In fluidized-bed applications where \( Re \) is \( O(10) \) or larger we expect that finite-\( Re \) correction to the fluid–particle drag force to become important. However, we expect even at finite \( Re \) that the anisotropy in the fluid–particle drag force will be qualitatively similar to the low-\( Re \) case. With this in mind, we restrict our attention in this study to low-Reynolds-number flows. (In contrast, the Stokes number is much larger than unity, which is assumed in the present study.) In the low-Reynolds-number limit, we express the friction coefficients in (2.18) and (2.19) as

\[ \beta = 18 \frac{\mu_e}{d^2} \phi (1 - \phi) F(\phi), \quad \hat{\beta} = 18 \frac{\mu_e}{d^2} \phi (1 - \phi) \hat{F}(\phi, Pe, \ldots) \]

(2.21)

where \( F(\phi) \) is a dimensionless friction coefficient, and \( \hat{F}(\phi, Pe, \ldots) \) is a dimensionless friction coefficient tensor. In § 4 we demonstrate the dependence of the elements of the friction coefficient tensor on \( Pe \), and subsequently link the changes in the fluid–particle drag to the microstructure of the particle assembly.
3. Simulation methods

3.1. Lattice-Boltzmann simulations

To isolate the effect of microstructural anisotropy on the fluid–particle drag force, our simulations were performed in two separate steps. First, we created anisotropic microstructures by performing constant-volume simple shear simulations of a granular system using the discrete-element method in the large-scale atomic/molecular massive parallel simulator (LAMMPS) code that was developed at Sandia National Laboratories (Plimpton 1995). In order to ensure that the simple shear deformation of the particle assembly was homogeneous, the simulation domain was continuously deformed, and gravitational effects were not included. The simulations were initiated by depositing a number of rigid particles into a periodic box, and allowing the particle assembly to equilibrate to a random hard-sphere microstructure. Subsequently, the particle assembly was sheared, as illustrated in figure 1, for a strain in excess of unity in order to ensure that the particle microstructure had reached steady state, following earlier work of Sun & Sundaresan (2011). For all of the fluid–particle drag results presented in this work, the $x$-, $y$- and $z$-components refer to the mean flow, vorticity, and gradient direction, respectively. At each time step in the shear deformation, the average particle fluctuation was calculated, and adjusted to reflect the desired fluctuating velocity specified by the user. In this way, the magnitude of the particle fluctuating velocity was controlled during the deformation, thus facilitating the creation of microstructures with different $Pe$ associated with the deformation. At each Péclet number and particle volume fraction, 16 different sheared particle configurations were created by shearing separate isotropic homogeneous assemblies created with different random seedings. Such a large number of realizations was required to ensure good statistical averages of the elements of the friction coefficient tensor.

The second step in the simulation procedure consisted of performing lattice-Boltzmann simulations of fluid flow through the anisotropic assembly of spheres. For our calculations we used the lattice-Boltzmann code developed by Tony Ladd for the simulation of particulate suspensions (Ladd 1994a,b; Ladd & Verberg 2001). The unique feature about the lattice-Boltzmann method is that it solves the evolution of a simplified particle velocity distribution function on a fixed lattice rather than solving
the Navier–Stokes equations directly (Chen & Doolen 1998; Ladd & Verberg 2001). The propagation and relaxation of the simplified particle velocity distribution function is designed such that the Navier–Stokes equations are reproduced on large length and time scales (Chen & Doolen 1998). In our simulations a 19-point quadrature in velocity space was used (D3Q19 method) giving a fluid density $\rho_g = 36$ in lattice units. In all simulations presented in this work the fluid viscosity $\mu_g = 6$ in lattice units. Previous work performed with the lattice-Boltzmann code of Ladd has shown that there is a substantial dependence of the fluid–particle drag results on the size of the particle used (van der Hoef, Beetstra & Kuipers 2005). In order to obtain fluid–particle drag results that were independent of size of the particle (i.e. grid resolution) used, an extrapolation as a function of the hydraulic radius $r_h = d(1 - \phi)/6\phi$ was performed (van der Hoef et al. 2005). In this study all simulations were performed with $d = 16.2$ lattice units in the cubic domain with $160^3$ grid points. Simulations were performed at particle volume fractions of $0.20, 0.30, 0.35, 0.40$ and $0.45$ where $351, 526, 614, 701$ and $798$ particles were used for each realization, respectively. At such high grid resolutions and fluid viscosities we find our results to be independent of grid resolution, therefore we do not perform an extrapolation of our fluid–particle drag results. The Reynolds number $Re = \rho_g d |u - v|/\mu_g < 0.02$ in the results presented here.

One can envision two different methods to simulate the fluid flow through anisotropic homogeneous assemblies of spherical particles. In the first method, snapshots of deformed particle microstructure and particle velocities in the periodic domain are imported from LAMMPS into the lattice-Boltzmann simulation, and fluid flow simulations are performed by freezing the positions of the particles (even though their velocities are non-zero) and applying a pressure gradient; this is a good approximation for large-$St$ and low-$Re$ systems (van der Hoef et al. 2005). In the second method of simulation, only the particle positions are imported while setting their velocities to zero, and fluid flow simulations are then performed in this fixed bed. The friction coefficient tensors obtained in these two types of simulations were within 1% of one another. All fluid–particle drag results presented in future sections were obtained using the second method of lattice-Boltzmann simulation discussed in this paragraph.

To determine the friction coefficient tensor, three simulations were performed with each snapshot, applying a pressure gradient in the three directions one at a time. The fluid–particle drag force from each realization was obtained by integrating the traction over the surface of all the particles in the simulation domain.

3.2. Continuum model simulations

The continuum model simulations presented in this work were performed using the Multiphase Flow with Interface eXchanges (MFIX) software (Syamlal 1998). The MFIX software is a finite-volume solver employing a variable time step and staggered grid to solve single- and multi-phase flow problems. Owing to the strong coupling between solid and fluid phases in gas–particle flows, the partial elimination algorithm of Spalding (1980) is used to decrease the coupling between the motion of the solid and fluid phases. To prevent spurious oscillations near the boundaries of clustered and dilute regions, the Superbee flux limiter is employed for all convective fluxes in our simulations. The Superbee flux limiter is a second-order-accurate scheme thereby ensuring that numerical diffusion effects are kept at a minimum. All two-fluid model simulations presented in subsequent sections were performed in two-dimensional doubly periodic domains where the particle assemblies were suspended by imparting a pressure gradient that exactly balances the weight of the suspension.
4. Fluid–particle drag in sheared assemblies

In assemblies subjected to simple shear as illustrated in figure 1, the friction coefficient tensor was found to be essentially symmetric, and the \( xy \)- and \( yz \)-components were found to be zero within the uncertainty of the measured friction coefficient. Figure 2(a–d) illustrates the variation of the remaining four components (scaled by the diagonal entries at \( Pe = 0 \)) for a particle volume fraction of 0.45. (Simulations were also performed at volume fractions of 0.20, 0.30, 0.35 and 0.40; the same trends as shown in figure 2 were obtained at all these volume fractions.) The \( xx \)-component manifests only a weak dependence on \( Pe \), while the other three shown in figure 2 reveal much larger variations. At \( Pe > 100 \), the friction coefficient tensor becomes essentially independent of \( Pe \). In the Appendix, an analysis is presented that links that value of the Péclet number to particle level properties by appealing to the kinetic theory of granular flow. Also, results from finite-volume simulations of (2.1)–(2.5) are presented where the spatial variation in the Péclet number is calculated.
Effect of microstructural anisotropy

Figure 3. (Colour online) Greyscale plots of the two-dimensional projection of the radial distribution function in the (a) $xy$-plane, (b) $xz$-plane and (c) $yz$-plane at three different values of $Pe$ for a particle volume fraction of $\phi = 0.45$.

In a heterogeneous gas–particle flow. These analyses reveal that $0 < Pe < 50$ is a reasonable range for fluidized beds, and hence further discussion is limited to only this range which is before the high-$Pe$ plateau. From the insets of figure 2(b–d) we note that at a value of $Pe \sim 50$ each element of the friction coefficient tensor has nearly reached its respective high-$Pe$ plateau.

In figure 3 we show a montage of the two-dimensional projection of the radial distribution of particles in $xy$-, $xz$- and $yz$-planes for three different values of $Pe$ at a particle volume fraction $\phi = 0.45$. The change in the particle microstructure is apparent as $Pe$ is increased. In the $xz$-plane a surplus of particles accumulates near the compressional axis of the simple shear deformation, while a depleted region is formed on the extensional axis of the shear flow. The depleted regions on the extensional axis of the simple shear deformation provide low-resistance ‘channels’ for the fluid to flow through, thereby decreasing the ensemble averaged $\beta_{yy}$ value.
It is clear that the changes in the observed fluid–particle drag force arise from variations in the particle microstructure from an isotropic random array of spheres. The microstructure tensor, $Y$, is written as (Stickel, Phillips & Powell 2006)

$$Y = \zeta_s I + Z,$$

$$\zeta_s = \frac{1}{4\pi} \int_{\Omega} \frac{a}{l_{mf}(\hat{x})} \, d\Omega,$$

$$Z = \frac{1}{4\pi} \int_{\Omega} X(\hat{x}) \frac{a}{l_{mf}(\hat{x})} \, d\Omega,$$

$$\lambda = \zeta_s^{-1}.$$

In (4.2), $\zeta_s$ is the particle radius scaled by the mean free path averaged over the solid angle $\Omega$, $l_{mf}(\hat{x})$ is the mean free path associated with a given direction $\hat{x}$, $\lambda$ is the mean free path averaged over all solid angles scaled by the particle radius, and $X(\hat{x})$ is the traceless dyadic product of $\hat{x}$ given as

$$X(\hat{x}) = \sqrt{\frac{15}{2}} \begin{bmatrix} \hat{x}_s\hat{x}_s - 1/3 & \hat{x}_s\hat{x}_y & \hat{x}_s\hat{x}_z \\ \hat{x}_s\hat{x}_y & \hat{x}_y\hat{x}_y - 1/3 & \hat{x}_y\hat{x}_z \\ \hat{x}_s\hat{x}_z & \hat{x}_y\hat{x}_z & \hat{x}_z\hat{x}_z - 1/3 \end{bmatrix}.$$

Deviations of the angle-averaged mean free path from the isotropic value, and changes in the off-diagonal components of the microstructure tensor from zero are related to the level of anisotropy of the particle assembly, which is directly related to $Pe$. Here we define

$$\lambda_{res} = \frac{\lambda - \lambda_0}{\lambda_0},$$

where $\lambda_0$ is the mean free path scaled by the particle radius for an isotropic system. Figure 4(a,b) illustrates that $\lambda_{res}$ and $Y_{xz}/\phi$ for the deformed particle assembly can be expressed functions of $Pe$.

### 4.1. Fluid–particle drag model

We express the friction coefficient tensor

$$\hat{\beta} = \beta I + \beta_1, \quad \beta_1 = \hat{\beta}_1 I + \hat{\beta}_1,$$

$$\hat{\beta}_1 = \frac{18}{d^2} \phi (1 - \phi) \hat{F}_1(\phi, Pe), \quad \hat{\beta}_1 = \frac{18}{d^2} \phi (1 - \phi) \hat{F}_1(\phi, Pe),$$

Figure 4. (Colour online) The connection between particle microstructure and changes in $Pe$ is illustrated by: (a) a plot of $\lambda_{res}$ versus $Pe$; and (b) a plot of $Y_{xz}/\phi$ versus $Pe$. 
where $\beta_1$ represents the anisotropic friction coefficient tensor which is partitioned into an isotropic part $\hat{\beta}_1$, and a deviatoric part $\tilde{\beta}_1$. $\tilde{F}_1(\phi, Pe)$ and $\hat{F}_1(\phi, Pe)$ are dimensionless and must be modelled. We propose a model for $\hat{F}_1$ as

$$
\tilde{F}_1(\phi, Pe) = \chi_1(\phi, Pe)\hat{S} + \chi_2(\phi, Pe)\left(\hat{S} \cdot \hat{S} - \frac{1}{3}(\hat{S} \cdot \hat{S})I\right) + \chi_3(\phi, Pe)(\hat{S} \cdot \hat{W} - \hat{W} \cdot \hat{S}),
$$

(4.6)

where $\hat{S}$ and $\hat{W}$ are rate-independent traceless deformation rate, and vorticity tensors, respectively, which are given as

$$
\hat{S} = \frac{S}{\sqrt{E:E}}, \quad \hat{W} = \frac{W}{\sqrt{E:E}},
$$

(4.7)

and are used to represent the kinematic effect of the shear deformation. In (4.6), $\chi_1(\phi, Pe)$, $\chi_2(\phi, Pe)$ and $\chi_3(\phi, Pe)$ represent the three model constants that constitute the deviatoric part of anisotropic friction coefficient tensor. In this model, $\chi_1$ and $\chi_2$ are introduced to capture the $\beta_{xz}$ and $\beta_{yy}$, respectively, in simple shear; $\hat{F}_1$ and $\chi_3$ then allow us to model observed $\beta_{xx}$ and $\beta_{zz}$. It should also be noted that in (4.6) the second and third terms on the right-hand side do not depend on the direction of shear deformation, while the first term does. This was deliberately done because the off-diagonal friction coefficient $\beta_{xz}$ was observed to change sign upon reversing the direction of shear, while the diagonal components of the friction coefficient tensor remained unchanged.

Figure 5 shows the variation of model parameters with the microstructural parameters. Figure 5(a–c) reveals that $\tilde{F}_1\phi^3/F$, $\chi_2$ and $\chi_3\phi^2$ correlate with $\lambda_{res}$ and $\phi$, while figure 5(d) shows that $\chi_1$ is a function of $Y_{xz}/\phi$. Based on figures 4 and 5, we arrive at the following correlations for the four model parameters:

$$
\hat{F}_1 = \frac{0.01}{\phi^3} F\lambda_{res}^2,
$$

(4.8)

$$
\chi_1 = 1.51 \left(1 - \exp \left(-1.17\frac{|Y_{xz}|}{\phi}\right)\right),
$$

(4.9)

$$
\chi_2 = 1.54 \left(1 - \exp \left(12.67\frac{\lambda_{res}\phi}{\phi}\right)\right),
$$

(4.10)

$$
\chi_3 = -\frac{0.097}{\phi^2}/\lambda_{res}^{4/3}.
$$

(4.11)

The microstructural variables in figure 4 can be related to $Pe$ as follows:

$$
\lambda_{res} = 0.073 \left(1 - \frac{1}{1 + 0.925 \left(\exp \left(-0.0422Pe - 1\right)\right)}\right),
$$

(4.12)

$$
|Y_{xz}| = 0.016\phi \left(Pe + 2.13 \times 10^{-4}Pe^3\right).
$$

(4.13)

For small-$Pe$, the fitting functions given in (4.8)–(4.13) reduce to the following:

$$
\hat{F}_1 \sim \phi^{-3/2}Pe^2, \quad \chi_3 \sim \phi^{-2}Pe^{3/2},
$$

(4.14a)

$$
\chi_1 \sim Pe, \quad \chi_2 \sim \phi Pe.
$$

(4.14b)

In (4.8) any isotropic drag model can be used for $F$. We found that the relationship proposed by van der Hoef et al. (2005) for low-$Re$ flows through random arrays given as

$$
F(\phi) = \frac{10\phi}{(1 - \phi)^2} + (1 - \phi)^2(1 + 1.5\sqrt{\phi}),
$$

(4.15)
agrees with our simulation results to within 1%. It should also be noted that the drag relation developed by Koch & Sangani (1999) describes our drag results equally well. Equation (4.15) is invoked in the linear stability analysis presented in the next section.

5. Discussion

5.1. Linear stability analysis
From inspection of figure 2 it can readily be seen that by imposing simple shear deformation in the plane perpendicular to gravity, one can alter the sedimentation velocity of a homogeneous suspension by up to $\sim 10\%$. In horizontal transport of non-neutrally buoyant suspensions, where velocity gradients naturally arise, the rates of sedimentation (or rise) of heavier (lighter) particles predicted by the isotropic and anisotropic drag models will differ. However, both of these effects are relatively small. In contrast, a more striking effect of the anisotropic drag model is observed in the classical problem of stability of uniform fluidization (sedimentation), which is discussed below.
We probe the effect of the anisotropic friction coefficient on the stability of the uniformly fluidized state by performing a linear stability analysis in one and two dimensions, and comparing dispersion relations for both isotropic and anisotropic drag models. Our analysis is based on (2.1)–(2.5). The governing equations are made dimensionless using \( u_c^2/g, u_t/g, u_t, u_t^2 \) and \( \rho_s u_t^2 \) as the characteristic length, time, velocity, temperature and pressure scales, respectively. For a uniformly fluidized state, (2.1)–(2.5) reduce to the following set of equations for particles that undergo elastic collisions:

\[
\phi = \phi_0 = \text{const}, \\
-2\phi_0 (1 - \phi_0) \frac{Fr}{St} F(\phi_0) \tilde{u}_0 - (1 - \phi_0) \left( \frac{1}{\delta} - \frac{\partial \tilde{p}_0}{\partial \tilde{x}} \right) = 0, \\
2\phi_0 (1 - \phi_0) \frac{Fr}{St} F(\phi_0) \tilde{u}_0 - \phi_0 \left( 1 + \frac{\partial \tilde{p}_0}{\partial \tilde{x}} \right) = 0, \\
\tilde{T}_0 = \left( \frac{\mathcal{E}(\phi_0)}{16 \sqrt{\pi} g_0 St (1 - \phi_0)^2 F(\phi_0)^2 R_{\text{diss}}(\phi_0)} \right)^{2/3},
\]

where the subscript zero refers to the base state, \( Fr \) is the Froude number based on particle diameter defined as \( Fr = u_c^2/(gd) \), \( \tilde{u}_0 \) is the dimensionless slip velocity between solid and fluid phases at the base state, \( \tilde{p}_0 \) is the dimensionless base-state fluid pressure, \( \tilde{T}_0 \) is the dimensionless base-state granular temperature, and \( \delta = \rho_s/\rho_g \). In this section the \( x \)-direction points vertically upward while the \( z \)-direction is in the horizontal plane. Note that for the low-\( Re \) flows considered here, \( Fr = (1 - 1/\delta)St/2 \), and so the model parameters are simply \( St, \phi_0 \) and \( \delta \).

The perturbations to the particle volume fraction, particle- and fluid-phase velocities, fluid-phase pressure, and the granular temperature have the following form:

\[
\psi = \psi_0 + \psi_1,
\]

where \( \psi \) represents a generic field variable, \( \psi_0 \) is its value at the base state, and \( \psi_1 \) is a small perturbation variable of the form

\[
\psi_1 = \hat{\psi}_1 \exp(ik \cdot x) \exp(\sigma t),
\]

where \( \hat{\psi}_1 \) sets the amplitude, \( \hat{k} \) is the wavenumber vector associated with the perturbation, and \( \sigma \) is the growth rate of the perturbation. Inserting these perturbations into (2.1)–(2.5), and simplifying we obtain a set of linear algebraic equations in the coefficients \( \hat{\psi}_1 \). The resulting characteristic equation takes the form of a fifth-order polynomial for the growth rate \( \sigma \) as a function of the wavenumbers \( k_x \) and \( k_z \). Note that while \( Pe = 0 \) in the base state, it will be non-zero in the perturbed state. Terms involving \( (\partial \chi_1/\partial Pe)_0 \) will appear in the characteristic equation, but \( \hat{F}_1, \chi_2 \) and \( \chi_3 \) and their derivatives with respect to Péclet number do not. As a result, identical dispersion relations are obtained with isotropic and anisotropic drag models for one-dimensional perturbations in the vertical direction (\( \hat{k}_z \neq 0 \) and \( \hat{k}_z = 0 \), here \( \hat{k} = k v_t^2/g \)). It then follows that the region in the \( (St, \phi_0, \delta) \) space where the state of uniform fluidization is predicted to be unstable using an anisotropic friction coefficient will not be smaller than that obtained using the isotropic friction coefficient.

Figures 6(a) and 6(b) show the real part of the maximum dimensionless growth rate \( \hat{\sigma}_r (= \sigma_r v_t/g) \) as a function of \( St \) for three different particle volume fractions.
for the isotropic and anisotropic drag model, respectively. Figure 6(c,d) compares the corresponding wavelengths of the dominant instability in the vertical direction. When the isotropic friction coefficient is used in the analysis the uniformly fluidized state is unstable at large $St$ values, but below a threshold value that depends on particle volume fraction the uniformly fluidized state is predicted to be stable. In contrast, the uniformly fluidized state is found to be unstable at all $St$ values when the anisotropic friction coefficient is used in the analysis. At very large $St$ values, where both models predict instability, the growth rates and the dominant vertical wavelengths predicted with the isotropic and anisotropic friction coefficients are quantitatively similar.

While the isotropic drag model predicts a one-dimensional travelling wave having no horizontal structure as the dominant mode of instability in a uniformly fluidized suspension, we find that the dominant instability mode has two-dimensional structure when an anisotropic drag model is used. Figure 7 shows the ratio between $\hat{k}_z$ and $\hat{k}_x$ for the fastest growing instability predicted by the linear stability analysis with the anisotropic drag model developed in this study. At each of the three volume fractions shown in this figure, a vertically travelling wave having both transverse and vertical
Figure 7. The ratio between dimensionless transverse ($\hat{k}_z$) and parallel ($\hat{k}_x$) wavenumbers of the dominant instability mode is plotted against $St$ for three different particle volume fractions. Here, we illustrate the emergence of two-dimensional structure that arises due to anisotropy in the fluid–particle drag force.

structures is dominant at lower $St$ values and it transitions to a mode with little lateral structure at large $St$ values. The $St$ value at which this transition occurs increases with particle volume fraction.

In our stability analysis, the granular temperature has been assumed to be isotropic; Koch & Sangani (1999) allowed the mean-squared velocity fluctuations in the vertical direction to differ from those in the transverse direction and formulated a more elaborate set of equations, but employed an isotropic friction coefficient. The $St$ value at which the uniformly fluidized state became stable for a given particle volume fraction was lower in the work of Koch & Sangani (1999) than what we report in figure 6(a) as a result of their anisotropic granular temperature formulation. The influence of the anisotropic granular temperature, however, is only quantitative; in contrast, a qualitative change is seen in our studies upon introduction of an anisotropic friction coefficient.

It should be noted that the model analysed here is valid only for large Stokes numbers and hence the lower end of $St$ values shown in these figures is outside the scope of the model. However, we do note that recent work by Xu et al. (2009) has revealed that high-Stokes-number continuum models have been shown to give accurate predictions of volume fraction profiles, and mean and fluctuating velocities in shear flows down to $St \sim 15$ when compared to direct numerical simulations. Moreover, the impact of the anisotropic friction coefficient is observed even at $St > 1$ (see figures 6(c,d) and 7); hence, we believe that our observation that the inclusion of anisotropic friction coefficient removes the stability predicted by the isotropic friction coefficient model remains valid.

Secondary circulation cells have been observed in low-$St$ sedimentation (Segre et al. 2001; Guazzelli & Hinch 2011). These have been rationalized in terms of particle volume fraction fluctuations that are always present in homogeneous sedimentation (Segre et al. 2001) and small gradients in vertical volume fraction (Mucha et al. 2004). It will be interesting to see if an anisotropic friction
coefficient has any role in inducing these circulation cells and/or the wavelength selection.

5.2. Two-fluid model simulation results

Another way to probe the effect of an anisotropic fluid–particle drag coefficient on two-fluid model predictions is to perform fully nonlinear finite-volume simulations of the two-fluid model with the anisotropic fluid–particle drag model developed in this work. Owing to the computational demand associated with fine-grid continuum model simulations, we limit the scope of our investigation to two-dimensional periodic-domain simulations. Since the simulations are restricted to a plane, a simplified form of the anisotropic fluid–particle drag model is employed, namely

\[ \tilde{F}_1(\phi, Pe) = \chi_1(\phi, Pe) \hat{S}. \] (5.7)

Comparing (5.7) with (4.6), it is clear that terms involving \( \chi_2 \) and \( \chi_3 \) have been neglected. This simplification was employed because the primary function of the \( \chi_2 \) and \( \chi_3 \) terms is to capture changes in the diagonal elements of the friction coefficient tensor for the case of simple shear. Any changes in the fluid–particle drag force in the vorticity direction will not be captured in two-dimensional simulations. Since the most substantial change to the diagonal elements of the drag coefficient tensor was observed in the vorticity direction (see figure 2b), with other changes being of secondary importance, we neglect terms \( \chi_2 \) and \( \chi_3 \) to simplify the analysis. However, it should be noted that three-dimensional, two-fluid model simulations should employ the definition of \( \tilde{F}_1 \) given in (4.6).

Instantaneous snapshots of the volume fraction field at statistical steady state are given in figure 8 for two-fluid model simulations where the isotropic and anisotropic drag models are used. Figures 8(a), 8(c) and 8(e) show the predicted particle volume fraction fields that are obtained when an isotropic fluid–particle drag model is employed at a domain-averaged volume fraction of \( \langle \phi \rangle = 0.55 \) and Stokes numbers of \( St = 25, St = 50 \) and \( St = 215 \), respectively, while the resulting volume fraction fields obtained from two-fluid model simulations employing an anisotropic drag model are given in figure 8(b,d,f). Juxtaposition of the volume fraction fields in figures 8(a) and 8(b) show that the snapshots of the particle volume fraction fields are qualitatively different, with simulation results based on the anisotropic drag model manifesting coarser flow structures than simulations based on an isotropic drag model at \( St = 25 \). The same conclusion holds true at \( St = 50 \) and \( St = 215 \) when comparing figures 8(c) and 8(d), and 8(e) and 8(f) respectively. To compare more quantitatively the resulting volume fraction fields, the energy spectra of the volume fraction fluctuations are calculated as follows:

\[ \hat{\phi}(k, t) = \int (\phi(x, t) - \langle \phi \rangle) \exp(ik \cdot x) \, dx, \quad E_\phi(k) = \frac{1}{2} \langle \hat{\phi}(k)\hat{\phi}^*(k) \rangle, \] (5.8)

where \( \hat{\phi} \) is the Fourier transform of the volume fraction fluctuations, \( E_\phi \) is the energy spectrum of the volume fraction fluctuations, \( \langle \cdot \rangle \) are used to indicate a domain-averaged quantity, and \( k \) is the scalar wave vector defined as \( k = |k| \). The energy spectra averaged over snapshots of particle volume fraction at statistical steady state are given in figure 9(a–c) for a domain-averaged volume fraction of \( \langle \phi \rangle = 0.55 \) at three different Stokes numbers. Figure 9(a–c) shows that the energy spectra of the volume fraction fluctuations are nearly identical for both isotropic and anisotropic models at low wavenumbers for \( St = 25 \), \( St = 50 \) and \( St = 215 \), but at
Figure 8. (Colour online) Snapshots of the particle volume fraction field obtained from periodic domain simulations are presented for a domain-averaged particle volume fraction of $\langle \phi \rangle = 0.55$ at: (a) $St = 25$ with the isotropic drag model; (b) $St = 25$ with the anisotropic drag model; (c) $St = 50$ with the isotropic drag model; (d) $St = 50$ with the anisotropic drag model; (e) $St = 215$ with the isotropic drag model; and (f) $St = 215$ with the anisotropic drag model. These simulations were performed in a two-dimensional periodic domain measuring 16 cm $\times$ 16 cm using 512 $\times$ 512 grid cells. In these snapshots gravity is acting vertically downward.
Figure 9. The energy spectra of the volume fraction fluctuations $E_\phi$ are presented as a function of dimensionless, scalar wavenumber $\hat{k}$ for both isotropic and anisotropic drag models at a domain-averaged volume fraction of $\langle \phi \rangle = 0.55$ for: (a) $St = 25$; (b) $St = 50$; and (c) $St = 215$. Here $\hat{k} = ku^2 / |g|$.

At high wavenumbers, the energy spectra are consistently smaller in the case of the anisotropic drag model when compared to the isotropic model. This supports the qualitative observation that the gas–particle flow structures observed when using an anisotropic drag model are coarser than the flow structures observed when using an isotropic drag model. It should be noted that the degree of deviation between the energy spectra of the volume fraction fluctuations for isotropic and anisotropic drag models increases as Stokes number decreases and volume fraction increases. While we do observe coarser gas–particle flow structures in simulations using an anisotropic fluid–particle drag model, we note that the domain-averaged slip velocities obtained from simulations using isotropic and anisotropic drag models are quantitatively similar.

6. Summary

The results of a computational study of the anisotropy in the fluid–particle friction coefficient in sheared particle assemblies are described. A model for the anisotropic friction coefficient tensor under low-$Re$ conditions is presented (equation (4.5)) and the
The influence of an anisotropic friction coefficient on the stability of the uniformly fluidized state was probed through linear stability analysis of the two-fluid model equations. When the friction coefficient anisotropy is not included, the uniformly fluidized state is most unstable at high Stokes numbers to vertically travelling disturbances having no transverse structure, but below some threshold $St$ value which depends on the particle volume fraction it is predicted to be stable.

When the anisotropy is included, a qualitatively different result is obtained, and the stability predicted at low $St$ disappears. The uniformly fluidized state is now most unstable to vertically travelling disturbances having both vertical and transverse structures. The aspect ratio of the most dominant mode is a function of both $St$ and particle volume fraction. At high Stokes numbers, the most dominant mode has very little transverse structure (and so is nearly the same as that obtained with an isotropic friction coefficient), but at lower Stokes numbers the aspect ratio is predicted to be of the order of unity.

Comparison between two-fluid model simulations of moderate- to high-Stokes-number suspensions both with and without the anisotropic fluid–particle drag model reveals that simulations using an anisotropic drag model predict coarser gas–particle flow structures than the corresponding simulation using an isotropic drag model.

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Appendix

In § 2 the deformation of the particle microstructure was linked to the magnitude of the Péclet number $Pe$. Estimates of typical values of $Pe$ for large-Stokes-number suspensions can be obtained by utilizing the kinetic theory of granular materials (Gidaspow 1994; Fan & Zhu 1998; Jackson 2000) and also by directly simulating (2.1)–(2.5) with constitutive relations given by (2.7)–(2.15) using finite-volume methods. If we appeal to the balance equation for pseudothermal energy in a gas–particle flow given by (2.5), and examine the simplified case of homogeneous simple shear deformation of the particle phase, where particles interact through binary, elastic collisions only, then the partial differential equation given in (2.5) reduces to the following nonlinear algebraic equation:

$$\frac{\mu_s \dot{y}^2}{2} + \Gamma_{slip} - J_{vis} = 0,$$

with the constitutive equations for $\mu_s$, $\Gamma_{slip}$ and $J_{vis}$ given by (2.9)–(2.14). The nonlinear expression given by (A1) can be solved numerically once characteristic values for $|u - v|$, $\phi$, $\rho_s$ and $d$ are chosen. The characteristic scale for the relative velocity between fluid and solid phases in a large-Stokes-number suspension can be obtained by a homogeneous momentum balance of the solid phase in the direction of the relative flow.
Figure 10. The characteristic value of $Pe$ plotted as a function of $\phi$ for three different values of $\dot{\gamma}$ as predicted from kinetic theory of granular flow. The values of $Pe$ are given for fluidized catalytic cracking (FCC) particles fluidized by a gas with the following physical properties for solid and fluid phases: $d = 75$ $\mu$m, $\rho_s = 1500$ kg $m^{-3}$, $\rho_g = 1.3$ kg $m^{-3}$ and $\mu_g = 1.8 \times 10^{-5}$ kg $(m s)^{-1}$.

It is clear that depending on the value of $\dot{\gamma}$ the Péclet number can reach values of $O(10)$ when a gas–particle flow is subjected to homogeneous simple shear deformation. Hence, the microstructural anisotropy resulting from such large values of $Pe$ will have a
Effect of microstructural anisotropy

Figure 11. Three different colourmaps of $Pe$ for domain-averaged volume fractions of: (a) $\phi = 0.20$; (b) $\phi = 0.30$; and (c) $\phi = 0.40$. In these periodic-domain simulations the particle- and fluid-phase properties are as follows: $d = 75$ μm, $\rho_s = 1500$ kg m$^{-3}$, $\rho_f = 1.3$ kg m$^{-3}$ and $\mu_s = 1.8 \times 10^{-5}$ kg (m s)$^{-1}$, which give $St \approx 180$. These simulations were performed in a two-dimensional periodic domain measuring 64 cm × 64 cm using 512 × 512 grid cells. The box size scaled by the particle diameter in this simulation is $8.53 \times 10^5$, and the Reynolds number based on the single-particle terminal settling velocity is 1.4. Gravity is acting vertically downward.

substantial impact on the fluid–particle drag force, and subsequently on the predictions of these two-fluid model equations.

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W. Holloway, J. Sun and S. Sundaresan


Effect of microstructural anisotropy


