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Momentum Transfer Between Polydisperse Particles in Dense Granular Flow

We perform molecular dynamics (MD) simulations (based on the soft-sphere model) of a model dry granular system consisting of two types of spherical particles differing in size and/or density to characterize particle-particle momentum transfer (solid drag). The velocity difference between two types of particles is specified in the initial conditions, and the evolution of relative mean velocity and the velocity fluctuations in terms of granular temperature are quantified. The dependence of the momentum transfer is studied as a function of volume fraction, size and density ratio of the two types of particles, inelasticity, and friction coefficient. An existing continuum model of particle-particle momentum transfer is compared to the MD simulations. A modified continuum solid drag model is suggested for a limited range of parameters. [DOI: 10.1115/1.2140803]

Introduction

Granular flows as well as dispersed particle flows (particles in fluid) are widely seen in nature and applied in industrial processes. Two approaches are currently used to model the motion of particle phase: particle (Lagrangian) approach and multiphase fluid model (continuum approach). In a particle approach, individual particles are tracked by solving for particle motion in a discrete element method (DEM) based on the soft-sphere contact model [1–3], which is popularly being called molecular dynamics (MD) [4,5] simulation in recent years. The capability of this approach is largely limited by the computational expense incurred in simulating a large number of particles. In a multiphase fluid model, the particle phase is approximated as a continuum fluid, and thus a set of continuum equations (conservation of mass, momentum, energy) for a control volume is obtained from granular gas kinetics. The advantage of the continuum approach is that it is capable of computing large systems. Particle number is not relevant in the continuum approach. One widely used numerical code, MFIX [6], developed at the National Energy Technology Laboratory (NETL), is based on the continuum approach, and this work is partially motivated by the modeling questions that arise during application of the code.

MFIX is a hydrodynamic model for fluid-solids flows, based on conservation laws of mass, momentum, energy, and species for describing the hydrodynamics, heat transfer, and chemical reactions in dense or dilute fluid-solids flows. The conservative equations must be closed by several constitutive relations including the particle-particle momentum transfer relation we are studying in this work. The model treats the fluid and solid phases as interpenetrating continua. Each solid phase consists of particles with identical particle properties such as density, diameter, and so on. Phase volume fractions are introduced to track the fraction of the averaging volume occupied by various phases. The code is used as a "test-stand" for testing and developing multiphase flow constitutive equations. More about MFIX can be found from the website of www.mfix.org.

The development of kinetic theory [7] of dense granular flows encounters a tremendous difficulty from the fact that particle collisions in granular flows are inelastic. The basic assumptions on which solving the Boltzmann equation [8] for ideal gas molecules (elastic collision) are based do not hold for granular flows. The continuum models have to be closed by employing approximations and empirical relations.

A real granular system consists of several kinds of particles with different sizes, densities, or other properties. For continuum models, each kind of particles is denoted as one solid particle phase and is described by one set of governing equations of continuum mechanics. Each particle phase has to experience internal "fluid-dynamics" [4,9], fluid-particle interaction, and particle-particle interaction, so that the fluid-particle momentum transfer term (also called fluid drag) and particle-particle momentum transfer term (also called solid drag) appear in the momentum equations of each particle phase. In this work, we focus on particle-particle momentum transfer through the study of a dry bidisperse granular mixture.

Existing models for particle-particle momentum transfer are semi-empirical and applicable to a limited range of flows [7] (dilute flows in most cases). In efforts to explore the characteristics of granular flows and enhance predictive ability of continuum models, lots of direct simulations of granular systems have been done. There are in general two methods in such MD simulations: soft-sphere model and hard-sphere model. The soft-sphere contact model is pioneered by Cundall and Strack [1]. In recent years several MD simulations of bidisperse granular systems [10,11] based on hard-sphere model are very attractive to the study of momentum transfer between particle phases.

In this work, we perform MD simulations of a dry bidisperse granular mixture in the soft-sphere framework [1–5] to characterize the solid drag for the simple system and compare the results to an existing continuum model, specifically the model used in MFIX (although other continuum models can also be used for comparison). We compare results from the two approaches, pro-

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pose a modified model based on the original MFIX model, and discuss ideas for improving the continuum model for solid drag.

Study System and Solution in Continuum Approach. A simple case, two types of dry particles in a control volume with periodic boundary conditions on all sides, and without external force, but with an initial velocity difference in one velocity component, is a good starting point for the study of particle-particle momentum transfer (or solid drag). The homogeneous and periodic conditions make the system simple for modeling in the continuum approach. The constitutive relations for dynamics inside a solid phase are not involved. In most continuum multiphase modeling [6], the governing equations for such a homogeneous case can be written as

$$\frac{d}{dt}(\epsilon_1\rho_1\mathbf{u}_1) = -F_{12}(\mathbf{u}_1 - \mathbf{u}_2) \tag{1}$$

$$\frac{d}{dt}(\epsilon_2\rho_2\mathbf{u}_2) = F_{12}(\mathbf{u}_1 - \mathbf{u}_2) \tag{2}$$

where $\epsilon_{1,2}$, $\rho_{1,2}$, $\mathbf{u}_{1,2}$ are the volume fraction, particle mass density, and number-weighted mean velocity for particles of type 1 and 2, respectively, and F_{12} is the solid drag coefficient. Due to the periodic conditions on all sides, the volume fractions in the control volume are fixed. Therefore, the velocity difference is obtained from the above equations as

$$\frac{d}{dt}(\mathbf{u}_1 - \mathbf{u}_2) = -\left(\frac{1}{\epsilon_1\rho_1} + \frac{1}{\epsilon_2\rho_2}\right)F_{12}(\mathbf{u}_1 - \mathbf{u}_2) \tag{3}$$

F_{12} is usually a linear function of magnitude of relative mean velocity in the form of

$$F_{12} = C_{12}|\mathbf{u}_1 - \mathbf{u}_2| \tag{4}$$

Here C_{12} is a coefficient that is independent of velocity. The governing equation then becomes

$$\frac{d}{dt}|\mathbf{u}_1 - \mathbf{u}_2| = -\left(\frac{1}{\epsilon_1\rho_1} + \frac{1}{\epsilon_2\rho_2}\right)C_{12}|\mathbf{u}_1 - \mathbf{u}_2|^2$$

The solution is

$$|\mathbf{u}_1 - \mathbf{u}_2| = \left[\left(\frac{1}{\epsilon_1\rho_1} + \frac{1}{\epsilon_2\rho_2}\right)C_{12}t + 1/|\mathbf{u}_1 - \mathbf{u}_2|_0\right]^{-1}$$

The system shares some properties with the homogeneous cooling state such as the asymptotic decay rate of the velocity is like $1/t$, a fact that follows from the lack of inherent time scales. For easy description of the current work, we normalize the solution using a velocity scale as the initial velocity difference $u_0 = |\mathbf{u}_1 - \mathbf{u}_2|_0/2.0$, a length scale as the average diameter of two types of particles $d_0 = (d_1 + d_2)/2$, and a time scale as $t_0 = d_0/u_0$. We use the notation u_{12} to denote the velocity difference $|\mathbf{u}_1 - \mathbf{u}_2|$ and $\tilde{C}_{12}$ to symbolize the term in dimensionless form, but we drop off the $\tilde{}$ on other terms such as velocity and time for simplicity. According to the MFIX model [6,12], we have the dimensionless momentum equation as well as its solution in our final form:

$$\frac{du_{12}}{dt} = -\tilde{C}_{12}u_{12}^2 \tag{5}$$

$$u_{12} = \frac{1}{\tilde{C}_{12}t + 0.5} \tag{6}$$

$$\tilde{C}_{12} = \left(\frac{1}{\epsilon_1\rho_1} + \frac{1}{\epsilon_2\rho_2}\right)\frac{d_1 + d_2}{2}C_{12} \tag{7}$$

$$C_{12} = \frac{3(1+e)(\pi/2 + \mu\pi^2/8)\epsilon_1\rho_1\epsilon_2\rho_2(d_1 + d_2)^2 g_0}{2\pi(\rho_1 d_1^3 + \rho_2 d_2^3)} \tag{8}$$

$$g_0 = \frac{1}{1 + \epsilon_s} + \frac{3d_1d_2}{(1 - \epsilon_s)^2(d_1 + d_2)}\left(\frac{\epsilon_1}{d_1} + \frac{\epsilon_2}{d_2}\right) \tag{9}$$

$$\epsilon_s = \epsilon_1 + \epsilon_2 \tag{10}$$

where e, μ are two microscale particle material properties during contacts: restitution and friction coefficient, ϵ_s is the total volume fraction of particles, $d_{1,2}$ is the particle diameter for particles of type 1 and 2, respectively, and g_0 is the radial distribution function at contact originated by Lebowitz [13].

It can be seen that the dimensionless solution is a function of e, μ, ϵ_1, ϵ_2, d_2/d_1, ρ_2/ρ_1, namely

$$\tilde{C}_{12} = f(e, \mu, \epsilon_1, \epsilon_2, d_1/d_2, \rho_1, \rho_2) \tag{11}$$

The solid drag coefficient is a function of many parameters. We cannot exhaust all the conditions to cover the full range of variation of every variable. In this work, we focus on the equal volume fractions of two particle phases and on medium to dense particle volume fraction.

The coefficient C_{12} in Eq. (8) is derived in MFIX [6,12] by considering two colliding particles located at $\mathbf{r}_1$, $\mathbf{r}_2$ with velocities $\mathbf{c}_1$, $\mathbf{c}_2$, and diameters d_1, d_2, respectively. The average momentum transfer per unit volume between the two types of particles is

$$\mathbf{I}_{12} = d_{12}^2\int_{\mathbf{c}_{12}\cdot\mathbf{n}>0}\mathbf{J}(\mathbf{c}_{12}\cdot\mathbf{n})f_{12}(\mathbf{r}_1, \mathbf{c}_1, \mathbf{r}_1 + d_{12}\mathbf{n}, \mathbf{c}_2)d\mathbf{n}d\mathbf{c}_1\mathbf{c}_2 \tag{12}$$

where $\mathbf{I}_{12}$ is average momentum transferred per unit volume, $d_{12} = (d_1 + d_2)/2$, the relative velocity $\mathbf{c}_{12} = \mathbf{c}_1 - \mathbf{c}_2$, $\mathbf{n}$ is the unit vector from the center of particle 1 to the center of particle 2, $\mathbf{J}$ is the momentum transferred between particles 1 and 2, and f_{12} is the pair distribution function which is assumed to be the product of two single velocity distribution functions

$$f_{12} = g_0 f_1 f_2 \tag{13}$$

The single velocity distribution functions take the form of a delta function

$$f_1 = 6\epsilon_1\delta(\mathbf{c}_1 - \mathbf{u}_1)/\pi d_1^3 \tag{14}$$

$$f_2 = 6\epsilon_2\delta(\mathbf{c}_2 - \mathbf{u}_2)/\pi d_2^3 \tag{15}$$

Following Walton [14], a collision is divided into sticking collision part and sliding collision part, so that the formulation of $\mathbf{J}$ will take into account the repulsion, dissipation, and friction effects.

Soft-Sphere MD Model. GranFlow is a parallel MD simulation code for granular flows that has been developed at Sandia National Lab. and has been evaluated, verified, and applied in many publications [3,5]. Readers who are interested in high-performance numerical algorithms are referred to Ref. [15]. The MD simulation is based on a 3D soft-sphere contact model [1–3] where small deformations and multiple contacts on a sphere are allowed, and friction and rotation are also taken into account. Contact force is first calculated from the deformation through a microscale spring-dashpot model, then is used in Newton's second law for every particle (spherical shape is assumed throughout this work) to update the velocity and angular velocity of each particle. The implementation of contact forces is essentially a reduced version of that employed by Walton and Braun [2], developed earlier by Cundall and Strach [1].

The spheres interact on contact through a Hookean (linear) contact law [1,2]. For two contacting particles $\{i, j\}$, at position $\{\mathbf{r}_i, \mathbf{r}_j\}$, with velocities $\{\mathbf{v}_i, \mathbf{v}_j\}$ and angular velocities $\{\boldsymbol{\omega}_i, \boldsymbol{\omega}_j\}$, a relative normal compression is

$$\boldsymbol{\delta}_{n,ij} = [(d_i + d_j)/2 - r_{ij}]\mathbf{n}_{ij} \tag{16}$$

where $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, $r_{ij}=|\mathbf{r}_{ij}|$ and the normal direction $\mathbf{n}_{ij}=\mathbf{r}_{ij}/r_{ij}$. The normal and tangential contact forces for particle i are given by

$$\mathbf{F}_{n,ij} = k_n\boldsymbol{\delta}_{n,ij} - \gamma_n m_{\text{eff}}\mathbf{v}_{n,ij} \tag{17}$$

$$\mathbf{F}_{t,ij} = -k_t\boldsymbol{\delta}_{t,ij} - \gamma_t m_{\text{eff}}\mathbf{v}_{t,ij} \tag{18}$$

where $m_{\text{eff}}=(m^i m^j)/(m^i+m^j)$, $\mathbf{v}_n$ and $\mathbf{v}_t$ are the normal and tangential components of the relative surface velocity, and $k_{n,t}$ and $\gamma_{n,t}$ are spring and damping coefficients, respectively. $\boldsymbol{\delta}_t$ is the elastic tangential displacement between spheres, obtained by integrating surface relative velocities over time during deformation of the contact. The magnitude of $\boldsymbol{\delta}_t$ is truncated as necessary to satisfy a local Coulomb yield criterion $|\mathbf{F}_t| \leqslant \mu|\mathbf{F}_n|$. Frictionless particles can be simulated by setting zero friction coefficient, $\mu=0$.

The presented simulations follow the same framework of Grest et al. [3,5] regarding the particle material parameters. The spring constants are set to $k_n=2\times10^5 m_* g/d_0$, where m_* and d_0 are mass and diameter of the particle in monodisperse mixtures, respectively, g is the gravity acceleration, and $k_t=2k_n/7$. The γ_n is related to restitution coefficient e. Such a correlation can be found in Ref. [3]. For a reference particle, physical experiments often use glass spheres of $d=100$ μm with $\rho=2\times10^3$ kg/m^3.

For the present polydisperse systems with two types of particles, when we investigate size or density effects, we wish to maintain contact parameters k_n, γ_n unchanged for better understanding and comparisons of results. For this purpose, the diameter and mass (or density) of a particle are varied proportionally relative to the corresponding particle. We maintain $d_0=(d_1+d_2)/2$ unchanged, so that d_0 is also equal to the diameter of particles when the two types of particle are the same.

The movement of particle i is described by Newton's second law in dimensionless form based on the normalization scales of m_*, d_0, g as

$$\frac{m_i}{m_*}\frac{d\mathbf{v}_i}{dt} = \sum_j \left(\tilde{k}_n\boldsymbol{\delta}_{n,ij} - \tilde{\gamma}_n\frac{m_{\text{eff}}}{m_*}\mathbf{v}_{n,ij}\right) + \sum_j \left(-\tilde{k}_t\boldsymbol{\delta}_{t,ij} - \tilde{\gamma}_t\frac{m_{\text{eff}}}{m_*}\mathbf{v}_{t,ij}\right) \tag{19}$$

$$0.4\frac{m_i}{m_*}\frac{d\boldsymbol{\omega}_i}{dt} = -\frac{1}{2}\sum_j d_i\mathbf{n}_{ij} \times \left(-\tilde{k}_t\boldsymbol{\delta}_{t,ij} - \tilde{\gamma}_t\frac{m_{\text{eff}}}{m_*}\mathbf{v}_{t,ij}\right) \tag{20}$$

The numerical simulation directly solves the above dimensionless equations, and input and output parameters are all in dimensionless form. We take $\tilde{k}_n=2\times10^5$, $k_t=2k_n/7$, and $\tilde{\gamma}_n=0,50$ (corresponding to $e=1,0.88$). For the Hookean contact model $\gamma_t=0$. Detailed discussion about contact parameters is available in Ref. [3].

To compare to a continuum model based on kinetic theory, the macroscopic terms (average variables) must be obtained from simulation results for the particle mixtures. The phase velocity $\mathbf{u}_{1,2}$ appearing in the continuum approach is equivalent to the average velocity over all particles of a type in the system. For example, for solid phase 1,

$$\mathbf{u}_1 = [u_1, v_1, w_1] = \sum_{i=1}^{N_1} \mathbf{v}_i/N_1 \tag{21}$$

N_1 is the number of particles of type 1. The granular temperature is defined as

$$\theta_1 = \sum_{i=1}^{N_1} [(u_i-u_1)^2 + (v_i-v_1)^2 + (w_i-w_1)^2]/3N_1 \tag{22}$$

where u_1, v_1, w_1 are three average velocity components. In this work, the volume of the simulation cell is $V=24^3 d_0^3$. The particle volume fractions for particle types 1 and 2 are calculated as

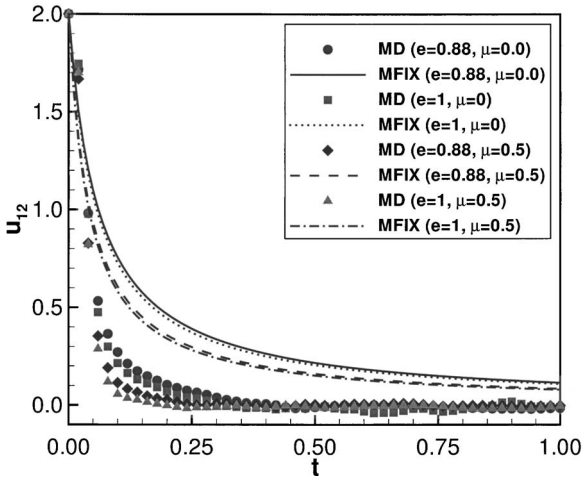

Fig. 1 Velocity difference u_{12} for $\epsilon_1=\epsilon_2=0.262$, $d_2/d_1=1/1$, and $\rho_2/\rho_1=1/1$

$$\epsilon_{1,2} = (\pi d_{1,2}^3 N_{1,2}/6)/V$$

Note that the normalization used here in simulations is different from that used in the previous section. The resultant terms of simulation must be transformed to the same normalization system on which the continuum model is based before any comparison is performed.

The particle mixture must be initialized to be spatially homogeneous. It is difficult to place all particles by random number generation methods, especially for dense mixtures. We use another way to initialize the system in this study. We first set all the particles in a form of lattice arrangements and assign an arbitrary velocity to each one, and then run the simulation to equilibrate the mixture. Because relative velocities of particles in a cooling system decay very fast, one run of the simulation may not result in the homogeneous condition. To ensure homogeneity, the output of a simulation is used as the input of particle positions to the next simulation, but the velocity of each particle is reset to a random value. The output-input procedure may be repeated several times. Finally, the input of particle positions from the homogeneous state is used to study cases with the velocity set to u_0 for one type of the particles and $-u_0$ for the other type.

Results and Discussion

Effects of e, μ, ϵ_s. The results are presented in dimensionless form and the units are omitted. The normalization scales have been given in the second section of deriving continuum solution of the granular system.

We first investigate the dependence of particle-particle momentum transfer on the total volume fraction and on the microscale properties e, μ. The particles in two phases are actually the same with $d_2/d_1=1$, $\rho_2/\rho_1=1$. Four combinations of $e=\{0.88,1\}$, $\mu=\{0.5,0\}$ are considered. According to the MD model, $e=1.0$ represents no energy loss during collision, $\mu=0$ represents no rotation.

The velocity differences u_{12} varying with time are plotted in Figs. 1 and 2, respectively, for total particle volume fraction $\epsilon_s=0.524$, 0.304. The initial momentum rapidly decays as the momentum of particles is redistributed isotropically through collisions (contacts). The granular temperature of the system immediately reaches its maximum. We can see the microscale parameters do make a difference on the momentum transfer, but the difference is relatively small compared with the difference between the MFIX model and MD simulation.

MFIX has captured the basic feature of contact parameters. The MFIX model follows the same trend as the MD simulations. The

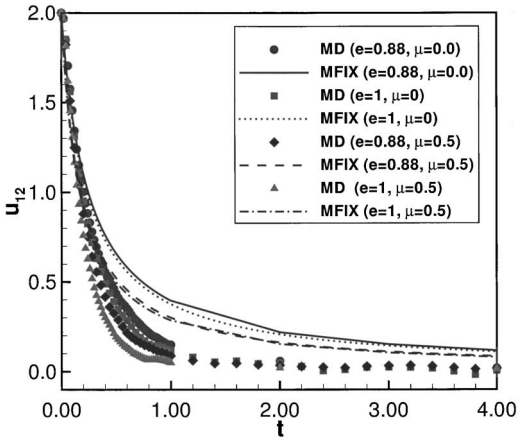

Fig. 2 Velocity difference u_{12} for $\epsilon_1=\epsilon_2=0.152$, $d_2/d_1=1/1$, and $\rho_2/\rho_1=1/1$

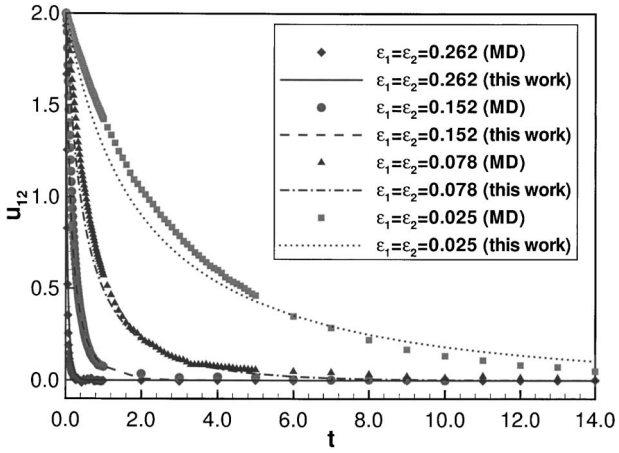

Fig. 4 Velocity difference u_{12} at various total volume fractions for $d_2/d_1=1/1$, $\rho_2/\rho_1=1/1$, $e=0.88$, and $\mu=0.5$

order of lines respective to different e, μ values from MFIX is the same as that from MD simulation. However, what concerns us most is the prominent gaps between the MFIX model and the MD simulation in Figs. 1 and 2, which overshadow the differences the microscale parameters make. It is clearly shown that the MFIX drag model underestimates the momentum transfer. Similar mismatches were observed for a wide range of total volume fractions. Agreement with the MFIX prediction becomes worse as the density of granular mixture increases.

The continuum solid drag model can be improved by separating the drag coefficient into two parts: a velocity-dependent part and a velocity-independent part as follows:

$$\frac{du_{12}}{dt} = -\tilde{C}_{12}u_{12}(1 + b/u_{12})u_{12} \tag{23}$$

The solution to this equation is

$$u_{12} = -b + b\left(1 - \frac{2.0}{2.0+b}\exp(-b\tilde{C}_{12}t)\right)^{-1} \tag{24}$$

In fact, we found that b is a function of total volume fraction ϵ_s, which is shown in Fig. 3. The curve fit gives the linear function

$$b = \epsilon_s + 0.42 \tag{25}$$

The model constant b is a correction to the original dilute granular flow solid drag model. Equation (25) indicates that the correction increases linearly with the total volume fraction.

The comparison of the suggested model and MD simulation for different volume fractions is shown in Fig. 4. The agreement is very good.

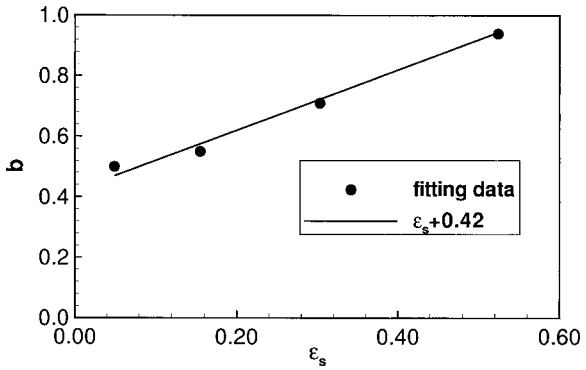

Fig. 3 b as a function of total volume fraction ϵ_s

Effects of Density Ratio. The velocity differences at different particle density ratios but with all other parameters the same ($e=0.88$, $\mu=0.5$, $\epsilon_1=\epsilon_2$, $d_1=d_2$) are plotted in Fig. 5. The results show that both MD and Eqs. (23)–(25) are not sensitive to variation of density. But, we must point out that the density effects could be important if the particle sizes are not the same, or the volume fractions of two particle phases are not equal, or the contact parameters change with the density. The present MD simulation uses the same contact coefficients for colliding particles, which deviates from the reality that material properties have much difference, especially when the densities are different.

Polydispersity. The size ratio plays a critical role in the solid drag model. This can be seen from the cubic power on particle diameters in Eqs. (7) and (8), but the drag model depends on other parameters only to the first power.

Figures 6–8 show the results for particles at different size ratios but with the same particle density $\rho_1=\rho_2$ and volume fraction $\epsilon_1=\epsilon_2=0.152$ for the case of $e=0.88$, $\mu=0.5$. The velocity difference u_{12} and granular temperature θ are plotted in Figs. 6 and 7, respectively. It is interesting to see that the phenomenon of momentum transfer between particle phases exhibits a nearly delta functional dependence on particle size. If the particle size ratio is just a little bit away from 1, specifically $d_2/d_1 \geqslant 1.1/0.9$, all the velocity difference curves settle down on nearly the same decay curve. However, near equal size, here $1 \leqslant d_2/d_1 \leqslant 1.05/0.95$, the velocity difference profiles are quite different from the group with

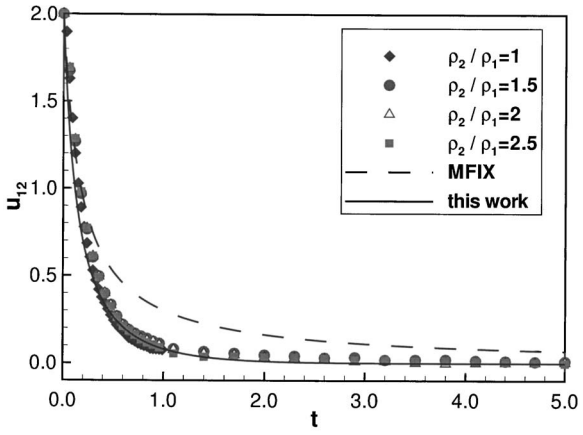

Fig. 5 Velocity difference u_{12} at various densities for $\epsilon_1=\epsilon_2=0.152$ and $d_2/d_1=1/1$

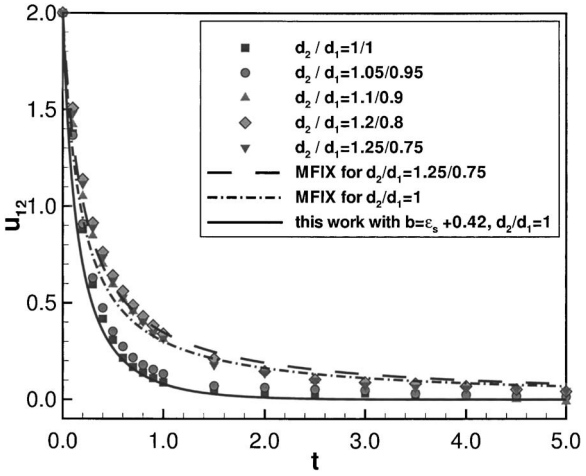

Fig. 6 Velocity difference u_{12} at different sizes for $e=0.88$, $\mu=0.5$, $\epsilon_1=\epsilon_2=0.152$, and $\rho_2/\rho_1=1$

$d_2/d_1 \geqslant 1.1/0.9$: they decay much faster than those with larger size ratios. From the comparison of the result of $d_2/d_1=1.1/0.9$ to that of $d_2/d_1=1.05/0.95$, we can see that a small change of particle size ratio results in a jump of velocity profiles between the two cases. But, in each group ($1 \leqslant d_2/d_1 \leqslant 1.05/0.95$ or $d_2/d_1 \geqslant 1.1/0.9$), the velocity profiles stay close together without obvious gaps among them.

It is encouraging to see that the agreement between Eq. (23) and MD simulation is very good for the particle size ratios which are a little bit away from 1, although the agreement is the worst at $d_2=d_1$. The suggested model of Eq. (23) still holds but needs further modification on b to address the particle size dependence issue:

$$\frac{du_{12}}{dt} = -\tilde{C}_{12}(1 + b/u_{12})u_{12}^2 \tag{26}$$

$$b = (\epsilon_s + 0.42)\left(\frac{d_{min}}{d_{max}}\right)^n \tag{27}$$

where d_{min} is the smaller diameter and d_{max} is the larger. In Eq. (27), the power n may need to be very large to account for the jump feature of solid drag. We found that $n=10$ gives satisfactory fit to the MD simulations.

As we have seen, the original MFIX modeling does not capture the discontinuity. So, the next question is what are the major contributors to the mismatch of the multiphase model with the MD

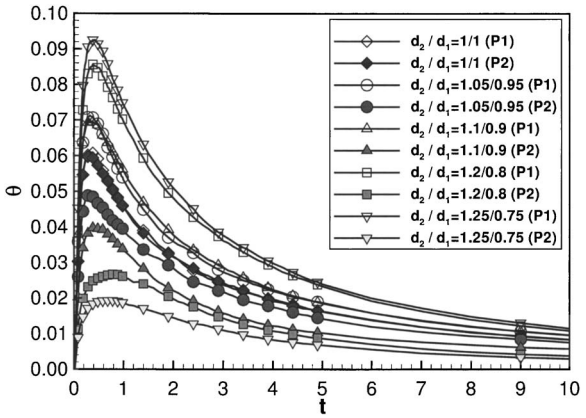

Fig. 7 Granular temperature θ at different sizes for $e=0.88$, $\mu=0.5$, $\epsilon_1=\epsilon_2=0.152$, and $\rho_2/\rho_1=1$. P1 denotes particle phase 1.

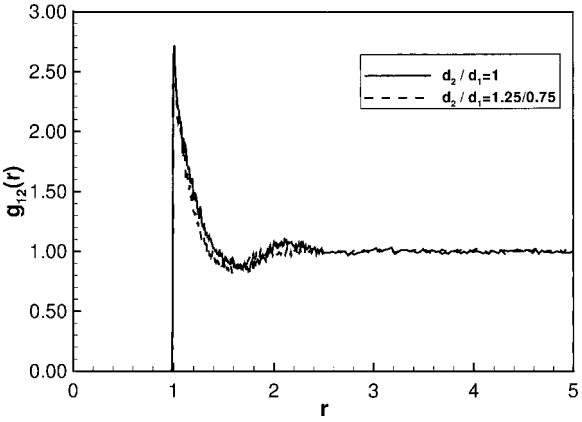

Fig. 8 Radial distribution function $g_{12}(r)$ for two cases of $d_2/d_1=1$ and $d_2/d_1=1.25/0.75$

simulation. The parameter g_0, the radial distribution function at contact, is worth studying. The MD simulation can be used to validate the independency at the specific conditions or to improve the form of g_0 since g_0 is the pair correlation function [16] that is equal to the radial distribution function $g_{12}(r)$ between particle types 1 and 2 evaluated at contact $r=d_0$.

The form of g_0 defined in Eq. (9) is originally from the work of Lebowitz [13]. Another form of g_0 was suggested by Mansoori et al. [17] and is known [18] to be more accurate. However, the inability of present models to predict particle-particle momentum transfer is not because of the form of g_0. As a matter of fact, both forms predict that g_0 is not a function of particle size ratio when the volume fractions of two phases are equal.

The pair velocity distribution function of two particles at contact is generally assumed in the term of product of two single particle velocity distribution functions [6,12,18], namely $f_{12}=g_0 f_1 f_2$. Thus, g_0 appears in the collision term calculation in kinetic theory.

In the case of spatially homogeneous systems as in the present study, $g_{12}(r)$ can be calculated by counting the pairs of separation [16] between particles of type 1 and particles of type 2 with $r-\delta/2 \leqslant |\mathbf{r}_{ij}| \leqslant r+\delta/2$. We use the numerical kernel function method [19] for this work. The g_0 relations given by Lebowitz [13] and Mansoori et al. [17] concern equilibrium states, but the study system in this work is dynamic at early times. We have calculated $g_{12}(r)$ of the granular assembly outputs from MD simulation at several moments. From the calculation, it is indeed found that $g_{12}(r)$ is statistically not a function of time as we expected, although fluctuations with time are found. We also found that the peak of $g_{12}(r)$ is not always exactly at contact distance, but at a slightly larger separation. Figure 8 gives the $g_{12}(r)$ averaged over five time points for two different particle systems. It shows the shape of $g_{12}(r)$ curves is weakly associated with particle sizes at $\epsilon_1=\epsilon_2$ condition. But, for both cases $g_0=g_{12}[(d_1+d_2)/2] \approx 2.5$. The form used in the MFIX model, Eq. (9), gives $g_0=2.37$.

Now, after g_0 has been excluded, we reason that a possible contributor to the disagreement is the assumed delta velocity distribution function during derivation [12] of the drag model in MFIX as shown in Eqs. (14) and (15). The largest momentum transfer happens when two identical particles collide. Due to the delta velocity distribution function, some of size information may be canceled out, leading to underestimation of the momentum transfer at the equal size condition. Other forms for the velocity distribution function could be checked against the simulations. Some models [18] use the Maxwellian distribution function or log-Maxwellian distribution function. Almost all continuous velocity distribution functions are functions of granular temperature in an effort to find out more accurate and general constitutive

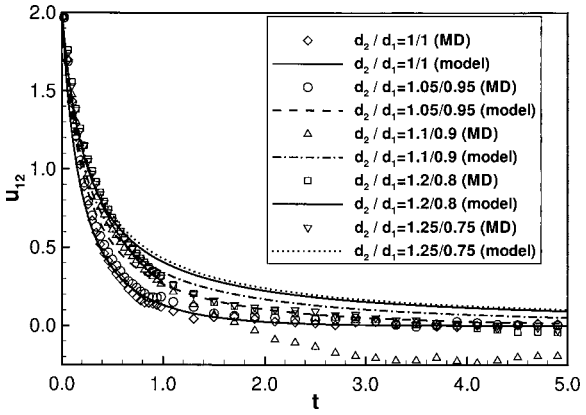

Fig. 9 Velocity difference at different sizes for $e=1.0$, $\mu=0$, $\epsilon_1=\epsilon_2=0.152$, and $\rho_2/\rho_1=1$ "model" means modified model in this work

relations. Note that when granular temperature is involved and a continuous distribution function applied, the near equilibration is often assumed from the point of view of kinetic theory. The application of such a model to a fast decay region starting with zero granular temperature needs to be examined, and the study system here may need to be redesigned in order to validate and explore continuum models.

To better understand the role of granular temperature, it may be helpful to consider frictionless elastic spheres ($e=1.0$, $\mu=0$). The results are shown in Figs. 9 and 10. Oscillation appears in the velocity difference profile when the relative mean velocity approaches zero, since the decay is due to the redistribution of energy in three directions, not to the energy loss. From the comparison of Fig. 9 with Fig. 6, we do see that granular temperature must play a role in the solid drag modeling formulation. For $e=1.0$, $\mu=0$, the velocity profiles from MD simulations diverge from the modeled curves after one time unit. Correspondingly, the granular temperatures increase from zero to the peaks in $t=[0,1]$ and remain at the peaks thereafter as shown in Fig. 10. However, granular temperatures rapidly decay after one time unit for the frictional and inelastic case $e=0.88$, $\mu=0.5$ as shown in Fig. 7. We will continue this work in the future. Note that a discontinuity feature like in Fig. 6 is always a difficult point for continuum modeling. Another discontinuity problem is referred to free-surface flows with surface tension on interfaces [20]. The discontinuity may imply some degree of crystallization at the equal size and equal volume fraction conditions. Away from the condition, crystallization is more unlikely to develop.

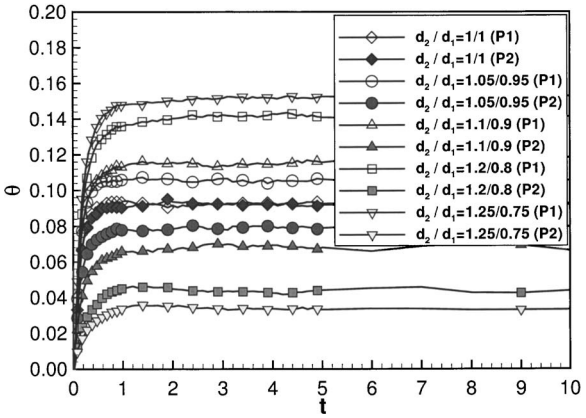

Fig. 10 Granular temperature θ at different sizes for $e=1.0$, $\mu=0$, $\epsilon_1=\epsilon_2=0.152$, and $\rho_2/\rho_1=1$. P1 denotes particle phase 1.

Conclusion and Future Work

We have investigated momentum transfer between particle phases in a limited range of variation of parameters from MD simulation and MFIX continuum drag model and have provided the comparison between them. We found a discontinuous behavior of particle-particle momentum transfer at equal particle sizes from the MD simulation. This discontinuity may point to some degree of crystallization at the condition of equal sizes and equal volume fractions and presents a difficulty in continuum modeling. The current MFIX model is in good agreement with the simulation when particle sizes are different, but underestimates the momentum transfer for particles of equal size. A tentative modified drag model based on the original MFIX model is proposed.

The current model of solid drag has not included the information of granular temperature due to an assumed delta velocity distribution function. Other solid drag models connecting to granular temperature should be considered and compared with simulation data in the future. At the same time, we also need to examine if the model is independent of initial conditions and whether implementation of initial conditions influences results. The study case may need redesign to avoid the zero granular temperature at the initial state. Moreover, all the cases we considered in this work have equal volume fractions for two particle phases. Further detailed study of two-particle phases with different volume fractions is encouraged, and the crystallization or discontinuity that happened at equal sizes and equal volume fractions may disappear. It is perhaps better to rewrite the dependence of solid drag on the governing parameters as

$$\tilde{C}_{12} = f(e, \mu, \epsilon_s, \epsilon_1/\epsilon_2, d_1/d_2, \rho_1/\rho_2) \tag{28}$$

Future work should give attention to the solid drag model varying with ϵ_1/ϵ_2. Indeed, the density ratio may not be negligible if $\epsilon_1 \neq \epsilon_2$. In addition, contact mechanics between different material particles should be taken into account in the MD simulation.

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