

The role of particle-particle interactions in bubbling gas-fluidized beds of Geldart A particles: A discrete particle study

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Abstract: Discrete particle simulations are by now well established as an effective tool to study the mechanics of complex gas-solid flows in gas-fluidized beds. In this study, a state-of-the-art discrete particle model is used to explore the role of particle-particle interactions in bubbling gas-fluidized beds of Geldart A particles. We find that the particle-particle interactions, including inelastic particle-particle collision; inter-particle friction and slightly cohesive forces, only have a negligible effect on the hydrodynamics of bubbling gas-fluidized beds of Geldart A particles. This is due to the fact that only a very small fraction of the energy input is dissipated during the non-ideal particle-particle interaction. We finally show that the selected drag correlation model significantly affects the bed hydrodynamics.

Keywords: Geldart A particles; Fluidization; Multiphase flow; Discrete particle simulation; Particle-particle interaction; Bubbling fluidized beds

1. Introduction

Bubbling fluidized beds (BFBs) are widely used in the petroleum, energy and chemical industries. Correct understanding of the hydrodynamic characteristics of BFBs is essential for design and scale-up of such reactors. However, the analysis of such system is very difficult, because of the coexistence of disparate length and time scales and the conspicuous coupling between the different scales with their transport properties (Li and Kwauk, 2003; van der Hoef et al., 2006). In order to obtain a fundamental insight into the complex hydrodynamics of BFBs, it is helpful to study the system from the basic interactions, i.e., the particle-particle interaction and the gas-particle interaction.

In recent decades, computer simulation has emerged as an effective tool to study the hydrodynamics of gas-fluidized beds (Gidaspow et al., 2004; Li et al., 2005; van der Hoef et al., 2008). Both Eulerian-Eulerian two-fluid model (TFM) and Eulerian-Lagrangian discrete particle model (DPM) are used to study the effect of particle-particle and gas-particle interactions on

the hydrodynamics of BFBs, however, most of them are devoted to Geldart B and D particles (for example, Goldschmidt et al., 2002; Goldschmidt et al., 2001; Hoomans et al., 1996; Li and Kuipers, 2003, 2007; Lu et al., 2005; Reuge et al., 2008; Wang et al., 2008; Xu et al., 2007). Those studies concluded that particle-particle interaction significantly affected the bed hydrodynamics. For example, based on two-fluid modeling with kinetic theory of granular flows (KTGF) for particulate phase stresses, Goldschmidt et al. (2001) showed that when the restitution coefficient equals one (i.e. ideal particles), no bubbling state is obtained for a fluidization velocity above three times the minimum bubbling velocity (which is equal to the minimum fluidization velocity for such a particle), whereas when a physically correct restitution coefficient is used, the bed hydrodynamics are predicted reasonably well by the TFM.

It is well-known that particle properties have a significant effect on the bed hydrodynamics (Geldart, 1973). Therefore, it is interesting to study what will happen when Geldart A particles are used as the bed material. Kobayashi et al.

(2002), Ye et al. (2004), Pandit et al. (2005; 2006) studied the effect of inter-particle cohesive forces on the homogeneous fluidization and the onset of minimum bubbling fluidization. However, only few studies are devoted to the hydrodynamics of Geldart A particles in BFBs, where all of them are based on TFM simulations. From those studies, a completely different picture as compared to B- and D-type particles emerged, namely, the restitution coefficient has no effect on the bubbling characteristics (Zimmermann and Taghipour, 2005), bed expansion characteristics (Wang et al., 2009b), minimum bubbling velocity and axial solid volume fraction profiles (Wang et al., 2009a). In these studies, the KTGF was used to represent the particle-particle interaction, which does include the effect of dissipation in collisions, but not the effect of particle-particle friction and/or inter-particle cohesive forces. So it remains as yet unclear how the latter two interactions will affect the bed hydrodynamics.

In this study, a state-of-the-art discrete particle model is used to explore the role of particle-particle interactions in BFBs of Geldart A particles. We show that the particle-particle normal restitution coefficient has a negligible effect on bed hydrodynamics, which confirm the results obtained from KTGF, we further find that the effect of particle-particle friction and slightly inter-particle cohesive forces are also negligible.

2. Discrete particle model

The DPM used here, which is pioneered by Tsuji et al. (1993) and Xu and Yu (1997), is part of the general multi-scale modeling strategy for numerical simulation of dense gas-solid fluidized beds (van der Hoef et al., 2008). The model has originally been developed by Ye et al. (2004), and is based on Hoomans et al. (1996). Below a summary of the main equations is given, details of the model can be found in Ye (2005) and van der Hoef et al. (2006).

In the DPM, the Eulerian grid size is usually far larger than the size of particles, so volume-

averaged Navier-Stokes equations are used to describe the motion of the gas phase. The mass conservation equation is given by

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = 0 \quad (1)$$

where ε_g , ρ_g and \mathbf{u}_g represent the local porosity, gas density and gas velocity vector, respectively. The momentum conservation equation is given by

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) \\ = -\varepsilon_g \nabla p - \mathbf{S}_p + \nabla \cdot (\varepsilon_g \bar{\bar{\tau}}_g) + \varepsilon_g \rho_g \mathbf{g} \end{aligned} \quad (2)$$

where p , \mathbf{S}_p , $\bar{\bar{\tau}}_g$ and \mathbf{g} are pressure, source term, shear stress tensor and gravitational acceleration, respectively, and $\bar{\bar{\tau}}_g$ is calculated from

$$\bar{\bar{\tau}}_g = \mu_g \left(\nabla \mathbf{u}_g + (\nabla \mathbf{u}_g)^T \right) - \frac{2}{3} \mu_g (\nabla \cdot \mathbf{u}_g) \bar{\bar{I}} \quad (3)$$

where μ_g and $\bar{\bar{I}}$ are shear viscosity of gas phase and unit tensor, respectively, and ρ_g is related to p through equation of state of an ideal gas

$$\rho_g = \frac{M_g}{RT_g} p \quad (4)$$

where R is the universal gas constant, T_g is the temperature and M_g is the molar mass of gas. The source term \mathbf{S}_p in Eq.2 is defined as

$$\mathbf{S}_p = \frac{1}{V_{cell}} \sum_{\forall a \in cell} \frac{\beta V_a}{1 - \varepsilon_g} (\mathbf{u}_g - \mathbf{v}_a) \delta(r - r_a) \quad (5)$$

where V_{cell} represents the volume of a computational cell, V_a the volume of particle a and \mathbf{v}_a the linear velocity of particle a . The δ -function ensures that the drag force acts as a point force at the central position of this particle. β is the inter-phase drag coefficient and is calculated by using the combined Ergun and Wen & Yu correlation (Gidaspow, 1994)

$$\beta_{Gidaspow} = \begin{cases} \frac{3}{4} C_D \frac{\rho_g \varepsilon_g \varepsilon_p |\mathbf{u}_g - \mathbf{v}_a|}{d_p} \varepsilon_g^{-2.65} & \varepsilon_p \leq 0.2 \\ 150 \frac{\varepsilon_p^2 \mu_g}{\varepsilon_g d_p^2} + 1.75 \frac{\rho_g \varepsilon_p |\mathbf{u}_g - \mathbf{v}_a|}{d_p} & \varepsilon_p > 0.2 \end{cases} \quad (6)$$

where $\varepsilon_p = 1 - \varepsilon_g$ and d_p are solid volume fraction and particle diameter, respectively, and C_D is calculated from the Schiller & Naumann expression,

$$C_D = \begin{cases} \frac{24}{\text{Re}_p} (1 + 0.15 \text{Re}_p^{0.687}) & \text{Re}_p < 1000 \\ 0.44, & \text{Re}_p \geq 1000 \end{cases},$$

$$\text{Re}_p = \frac{\varepsilon_g \rho_g d_p |\mathbf{u}_g - \mathbf{v}_a|}{\mu_g} \quad (7)$$

Note that in DPM, the porosity is calculated by

$$\varepsilon_g = 1 - \frac{1}{V_{\text{cell}}} \sum_{\forall a \in \text{cell}} f_a V_a \quad (8)$$

where $f_a V_a$ is the fractional volume of particle a residing in the cell under consideration.

The particle phase is described by the Newton equations of motion for each particle in the system. The translational and rotational equations of motion for a single particle a are given by

$$m_a \frac{d\mathbf{v}_a}{dt} = -V_a \nabla p + \frac{V_p \beta}{1 - \varepsilon_g} (\mathbf{u}_g - \mathbf{v}_a) + m_a \mathbf{g} + \mathbf{F}_{c,a} + \mathbf{F}_{vdw,a} \quad (9)$$

$$I_a \frac{d\omega_a}{dt} = \mathbf{T}_a \quad (10)$$

where m_a , I_a , ω_a , \mathbf{T}_a and t represent particle mass, moment of inertia, angular velocity, torque and time, respectively. The first and second terms in the right hand side of Eq.9 originate from inter-phase interaction. The third term is caused by gravity, the fourth term is the contact force resulting from particle-particle or particle-wall interaction, which is calculated using the soft-sphere model proposed by Cundall and Strack (1979). The fifth term is the inter-particle cohesive force, which is represented by using the van der Waals force ($\mathbf{F}_{vdw,a}$), and is given by

$$\mathbf{F}_{vdw,a} = \sum_{\forall b \in \text{Neighbourlist}} \mathbf{F}_{vdw,ab} \mathbf{n}_{ab} \quad (11)$$

$$\mathbf{F}_{vdw,ab} = -\frac{A}{3} \frac{2r_a r_b (S + r_a + r_b)}{[S(S + 2r_a + 2r_b)]^2} \times \left[\frac{S(S + 2r_a + 2r_b)}{(S + r_a + r_b)^2 - (r_a - r_b)^2} - 1 \right]^2 \quad (12)$$

where \mathbf{n}_{ab} is the normal unit vector, S is the inter-surface distance between two spheres, A is the Hamaker constant, and r_a and r_b are the radii of the two spheres. Note in our case $r_a = r_b$. To avoid the singularity when the distance between two particles approaches zero, we define a maximal value of the van der Waals force between two particles, which is realized by using a cut-off value for the inter-surface distance, S_0 .

In the numerical simulations, boundary and initial conditions have to be specified. At the top outlet, the pressure is specified as the atmospheric pressure (101325Pa), whereas at the bottom inlet, a uniform gas velocity profile with specific superficial gas velocity (U_g) is imposed, free-slip wall is applied for gas phase as in a previous study (Ye et al., 2005). The particles are initially packed at the bottom of the bed with zero average velocity plus a random fluctuating velocity. Note that in our simulations, the tangential restitution coefficient is always set equal to the normal restitution coefficient and the parameters for the particle-wall interaction are equal to the parameters for the particle-particle interaction.

3. Result and discussion

As in the available studies on two-fluid modeling of Geldart A particles in BFBs, we have focused on the effect of particle-particle interaction. Table.1 summarizes the parameters used in the simulations, which are similar to those in the study by Ye et al. (2005). Note that all of the simulations last 5s, the first second of which is used to equilibrate the system, and the remaining 4s (which are free of start-up effects) are used to measure the various quantities of

interest, which are sampled with a frequency of 10000Hz.

Table.1 A summary of the parameters used in the simulations

Parameters	Value
Particle number, N_{part}	36000
Particle diameter, d_p	$7.5 \times 10^{-5} \text{m}$
Particle density, ρ_p	1495kg/m^3
Restitution coefficient, e_n, e_t	0.6, 0.7, 0.8, 0.9, 1.0
Friction coefficient, μ_f	0.1, 0.2, 0.3, 0.4, 0.5
Normal spring stiffness, k_n	7 N/m
Tangential spring stiffness, k_t	2 N/m
CFD time step	$1.0 \times 10^{-5} \text{s}$
Particle dynamics time step	$1.0 \times 10^{-6} \text{s}$
Minimum inter-particle distance, S_0	0.4nm
Reactor height	$1.2 \times 10^{-2} \text{m}$
Reactor width	$3.0 \times 10^{-3} \text{m}$
Reactor depth	$1.2 \times 10^{-3} \text{m}$
Number of CFD cells	$48 \times 12 \times 5$
Gas temperature, T_g	293K
Gas constant, R	$8.314 \text{J}/(\text{mol} \cdot \text{K})$
Molar mass of gas, M_g	$28.8 \times 10^{-3} \text{kg/mol}$
Shear viscosity of gas, μ_g	$1.8 \times 10^{-5} \text{Pa} \cdot \text{s}$

Snapshots from a simulation of a typical bubbling fluidized bed ($U_g=0.04\text{m/s}$) are shown in Fig.1. There is no effect for different values of restitution coefficient (e), friction coefficient (μ_f) and Hamaker constant (A). From fig.1 (a), it can be seen that the normal particle-particle interaction does not affect the bubble characteristics, and even in case of $e=1$, bubbles can still be clearly detected, which is in agreement with previous simulation results for Geldart A particles using a two-fluid modeling (Wang et al., 2009a; Zimmermann and Taghipour, 2005), and is clearly different from the DPM results for coarse particles, where it was shown that particle collision properties have a profound effect on bed hydrodynamics, where in case of $e=1$, no two-phase structure emerges at all (Li and Kuipers, 2007).

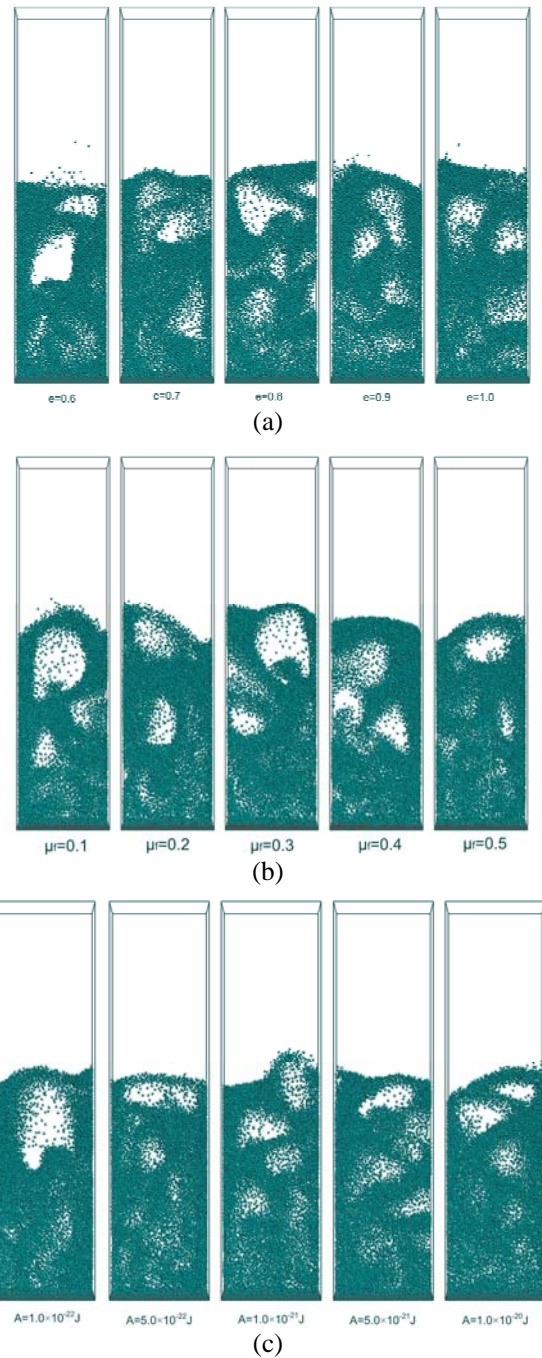
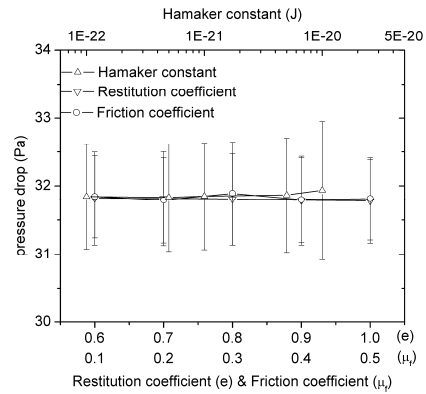


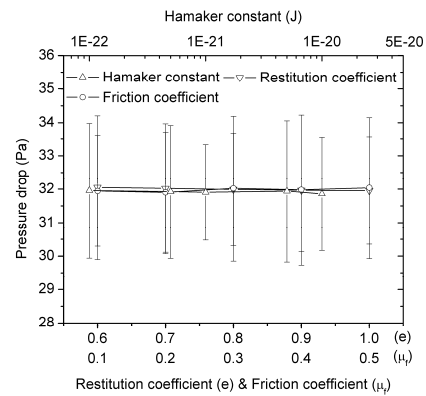
Figure.1 Snapshots of simulation results taken at a slit (the particles located at the dimensionless bed depth between 0.35 and 0.65 are shown). Showing the effect of restitution coefficient (a), friction coefficient (b) and Hamaker constant (c). $U_g=0.04\text{m/s}$. In (a) the inter-particle friction and cohesive forces are not included; in (b) $e=0.9$, the effect of cohesive force is not included; in (c) $e=0.9, \mu_f=0.3$.

By comparing fig.1 (a) with fig.1 (b), we conclude that the inclusion of the effect of inter-particle friction has no visible effect on the bed structures, which is again in strong contrast with the observations for coarse particles (Li and Kuipers, 2007). Fig.1 (c) indicates that within the ranges we studied, the effect of cohesive forces are negligible, which can be understood from the fact that the cohesive force is a short range interaction. Since the average porosity in our cases is about 0.6-0.7, the mean inter-particle distance is large, so the effect of van der Waals forces becomes extremely weak. However, it must be pointed out that the conclusion obtained here is somewhat different from one of our previous 2D DPM studies on Geldart A particles (Ye et al., 2004), where it was shown that when $A=10^{-20}$ J, chain-like structures are formed and the inter-particle cohesive force is the dominant source of the velocity fluctuation of particles.

A possible origin could be that the inter-particle cohesive force not only depends on the Hamaker constant but also on the inter-particle distance, and that for the same solid volume fraction and Hamaker constant, the inter-particle distance in 2D is less than in 3D, which means that the inter-particle cohesive force in 3D is weaker than the one in 2D. We can imagine that with decreasing U_g , the cohesive force will play an increasing role in the fluidization of Geldart A particles, however, we do not address this issue here, because (1) a large number of DPM simulations have already been devoted to homogeneous fluidization and the onset of minimum bubbling fluidization as stated in the introduction section; (2) the cohesive force used here hardly represents the true nature of inter-particle cohesive forces; and most importantly, (3) industrial gas-fluidized beds are seldom operated at such low superficial gas velocity.



(a)



(b)

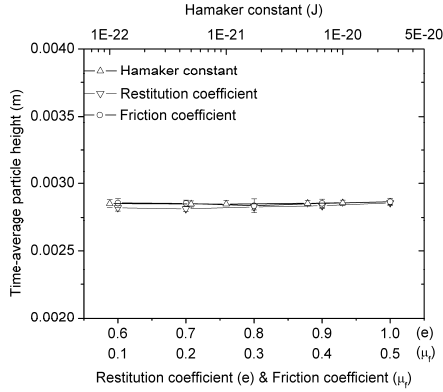
Figure.2 The effect of particle-particle interaction on the pressure drop and its deviation, (a) $U_g=0.02$ m/s; (b) $U_g=0.04$ m/s

Fig.2 shows the effect of particle-particle interaction on the pressure drop at $U_g=0.02$ m/s and $U_g=0.04$ m/s, respectively. It can be seen that particle-particle interaction does not affect the pressure drop and its standard deviation, which is again in contrast with the observations for coarse particles as reported by Li and Kuipers (2007), where it was shown that due to the significant change in the spatial and temporal structures caused by different particle-particle interaction characteristics, stronger collisional dissipation leads to stronger pressure oscillations.

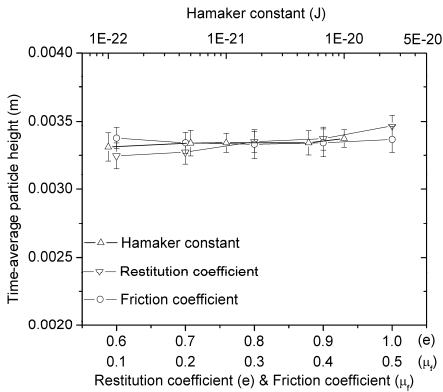
Also for the time-average particle height, the effect of the particle interaction is marginal as shown in fig.3, where the particle height is defined as (Goldschmidt et al., 2004)

$$\langle h_p \rangle_{bed} = \frac{\sum_{i=1}^{N_{part}} h_i}{N_{part}} \quad (13)$$

It worthwhile to mention that without the inclusion of particle friction and cohesive forces, a higher restitution coefficient results in higher time-average particle height. In case of a superficial gas velocity of 0.04m/s, the time-average particle height with $e=1$ is about 6% higher than the value obtained by using $e=0.6$. Since this variation is within the reported standard deviations of time-average particle height, we still conclude that particle-particle interaction has no pronounced effect on the time-average particle height.



(a)



(b)

Figure.3 The effect of particle-particle interaction on the time-average particle height, (a) $U_g=0.02\text{m/s}$; (b) $U_g=0.04\text{m/s}$

Fig.4 shows the effect of particle-particle interaction on the global granular temperature, which is defined as,

$$\Theta = \frac{1}{3}(\Theta_x + \Theta_y + \Theta_z) \quad (14)$$

where the granular temperature in the k -direction Θ_k , is defined as

$$\Theta_k = \frac{\sum_{i=1}^{N_{part}} (v_{k,i} - \bar{v}_k)^2}{N_{part}} \quad (15)$$

and the average velocity \bar{v}_k , is defined as

$$\bar{v}_k = \frac{\sum_{i=1}^{N_{part}} v_{k,i}}{N_{part}} \quad (16)$$

Note that this definition of granular temperature indicates that the effect of heterogeneous structures on the granular temperature is already included. It can be seen that all computed granular temperatures for same U_g are comparable. Since in BFBs, the granular temperature is dominated by the bubble structure (Campbell and Wang, 1991; Menon and Durian, 1997), this means that the bubble structure is not affected by the particle-particle interaction. Based on our results, we therefore conclude that for Geldart A particles, particle-particle interaction only plays a negligible role in the structure formation of BFBs.

It is as yet unclear why the role played by particle-particle interaction is negligible for Geldart A particles. Recently, a series of studies (Goldschmidt et al., 2004; Li and Kuipers, 2002, 2004, 2007) have revealed that energy budget analysis is a powerful tool to analyze the underlying mechanics of gas-solid flows. In Fig.5, we show the effect of restitution coefficient on the energy budget analysis at a superficial gas velocity of 0.04m/s without the presence of friction and cohesive forces. In fig.5, f_{kin} , f_{pot} , f_{sprn} and f_{dispn} represent the fraction of kinetic energy, potential energy, potential energy of the normal spring and energy dissipation by the normal spring of the total particle energy, respectively.

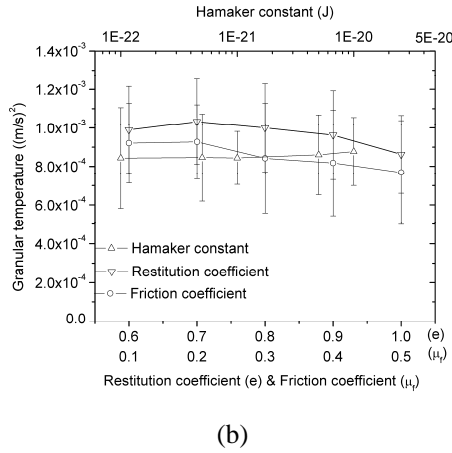
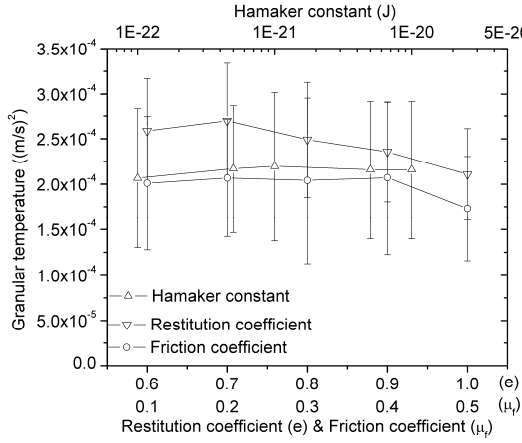


Figure.4 The effect of particle-particle interaction on the global granular temperature, (a) $U_g=0.02\text{m/s}$; (b) $U_g=0.04\text{m/s}$

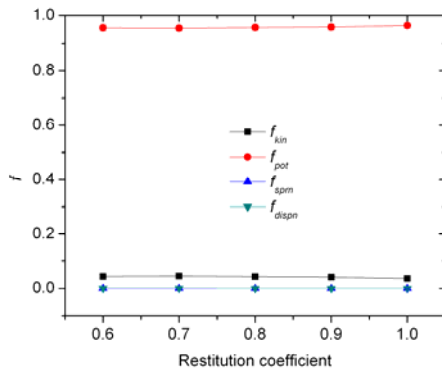


Figure.5 Energy budget analysis of particle phase, $U_g=0.04\text{m/s}$, without consideration of the effect of inter-particle friction and cohesive force.

Details of their mathematical expressions can be found in Ye (2005). Note that the results for

all cases are similar, therefore, for simplicity only the effect of restitution coefficient is shown. The energy budget analysis on the particle phase reveals that almost all of the energy input is used to keep the particles in suspension with a constant granular temperature (i.e. kinetic energy), only a very small fraction of the energy input (less than 1% in all cases we studied) is dissipated in the non-ideal particle-particle interactions.

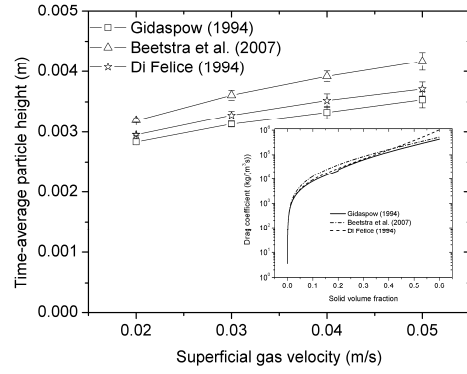


Figure.6 The effect of drag correlations on the time-average particle height, the inset shows the comparison of the drag coefficients by Ergun and Wen and Yu (Gidaspow, 1994), Di Felice (1994) and Beetstra et al. (2007) at an inter-phase slip velocity of 0.04m/s .

Finally, simulations are performed in order to study the effect of drag correlations. Two different drag correlations are considered, one which is obtained using lattice Boltzmann simulations (Beetstra et al., 2007),

$$\beta_{Beetstra} = 180 \frac{\mu_g \varepsilon_p^2}{d_p^2 \varepsilon_g} + 18 \frac{\mu_g \varepsilon_g^3 \varepsilon_p (1 + 1.5 \sqrt{\varepsilon_p})}{d_p^2} + 0.31 \frac{\mu_g \varepsilon_p \text{Re}_p \left[\varepsilon_g^{-1} + 3 \varepsilon_g \varepsilon_p + 8.4 \text{Re}_p^{-0.343} \right]}{\varepsilon_g d_p^2 \left[1 + 10^{3 \varepsilon_p} \text{Re}_p^{-0.5-2 \varepsilon_p} \right]} \quad (17)$$

and the other is developed by Di Felice (1994) which is widely used in DPM community:

$$\beta_{Felice} = \frac{3}{4} C_D \frac{\rho_g \varepsilon_p \left| \mathbf{u}_g - \mathbf{v}_a \right|}{d_p} \varepsilon_g^{-\chi} \quad (18)$$

$$C_D = \left(0.63 + \frac{4.8}{\sqrt{\text{Re}_p}} \right)^2,$$

$$\chi = 2.7 - 0.65 \exp \left[-\frac{(1.5 - \log_{10} \text{Re}_p)^2}{2} \right] \quad (19)$$

Fig.6 shows the effect of drag correlations on the time-average particle height with $e=0.9$ and $\mu_f=0.3$. It can be seen that the drag correlation has a profound effect on the time-average particle height. For example, for the case of a superficial gas velocity of 0.05m/s, the value simulated using the drag correlation of Beetstra et al. (2007) is about 18% higher than the one obtained using Gidaspow's correlation (1994). Even for a lower superficial gas velocity of 0.02m/s, the relative error is still larger than 12%. This is obviously due to the fact that the drag coefficient of Beetstra et al. (2007) is larger than the one by Gidaspow (1994) as shown in the inset of fig.6. However, because no corresponding experimental data is available, it is unclear which correlation is best for the simulation of Geldart A particles in BFBs. It should be born in mind that due to the limitation of computational resources, only a very small system can be simulated by DPM, so that, special experimental studies of micro-gas-fluidized beds are necessary to assess which correlation is the best.

4. Conclusion

A state-of-the-art discrete particle model is used to explore the role of particle-particle interaction in bubbling gas-fluidized beds of Geldart A particles. We find that in general particle-particle inelastic interactions do not affect the typical bed characteristics that we studied, such as the pressure drop and its standard deviation, the time-average particle height and the global granular temperature. This confirms the previous conclusion based on the two-fluid modeling of Geldart A particles with kinetic theory of granular flows for particulate phase stresses. We further show that the

presences of particle-particle friction and slightly cohesive forces also have a negligible effect, from which we conclude that particle-particle interaction only plays a negligible role in the hydrodynamics of bubbling gas-fluidized beds of Geldart A particles. Finally, we showed that the inter-phase drag correlation used, which reflects the gas-particle interaction in the DPM simulations, constitutes a control factor in the bed hydrodynamics.

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