DISCRETE PARTICLE SIMULATION OF THE HOMOGENEOUS FLUIDIZATION OF GELDART A PARTICLES

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ABSTRACT

The homogeneous fluidization of Geldart A particles has been studied with a 2D soft-sphere discrete particle model. We find that the homogeneous fluidization regime represents a quasi-equilibrium state where the force balance exists at the macroscopic-level, but not at the level of individual particles. The velocity fluctuation of particles is an exponential function of the squared superficial gas velocity in the homogeneous fluidization regime, not a linear function as found by Cody et al. (1).

INTRODUCTION

The significant practical relevance of the homogeneous fluidization of Geldart A particles (2) in gas-fluidized beds has long been recognized. Over the past years, the phenomenon of homogeneous fluidization has been a subject of intense research by engineers and scientists. However, most of the studies have been carried out at the macroscopic-level ignoring the details of particle-particle interaction and gas-particle interaction inside the fluidized beds.

Rietema and his co-workers (3,4) were among the researchers who argued that the particle-particle interactions, especially the interparticle van der Waals forces, are responsible for the homogeneous fluidization behavior of small particles. On the other hand, Foscolo and Gibilaro (5) argued that the hydrodynamic interaction between fluid and particles is the dominant factor that causes the instability of the homogeneous fluidization regime. Both groups were able to predict some important features of homogeneous fluidization, however, the phenomena associated with the homogeneous fluidization are not yet completely understood. To understand the combined effect of particle-particle interaction and gas-particle interaction thoroughly, computer simulation can play am important role.

The discrete particle model (DPM), in which the trajectories of individual particles are computed from the Newtonian equations, provides an efficient way to investigate the effect of the particle-particle interactions. Basically there are two kinds of discrete particle models, the hard-sphere model (6) and soft-sphere model (7,8). In this research, a soft-sphere discrete particle model (DPM) has been used to simulate the fluidization behavior of Geldart A particles, since (1) in the homogeneous fluidization there may exist multiple contacts between particles

and (2) it is relatively easy to incorporate the interparticle van der Waals force in soft-sphere model. Note that with such a detailed level of description, the size of the beds employed is relatively small. In this respect, the model should be regarded as a "learning" model. The information obtained from the discrete particle simulation will be used to increase our knowledge of the particulate pressure and viscosity and improve the two-fluid models, which are widely used to describe large-scale fluidized beds. In a recent paper (9), we have discussed the effect of interparticle van der Waals forces on the fluidization behavior of Geldart A particles. It has been shown that the homogeneous fluidization is a transition phase that results from the competition between the complex particle-particle interactions and gas-particle interaction. In this paper, we will further investigate the effect of particle-particle interactions on the homogeneous fluidization.

THEORETIC MODEL

The gas flow is modeled by the volume-averaged Navier-Stokes equations given by:

$$\frac{\partial\left(\varepsilon\rho_g\right)}{\partial t}+\left(\nabla\cdot\varepsilon\rho_g\mathbf{u}\right)=0 \tag{1}$$

$$\frac{\partial\left(\varepsilon\rho_g\mathbf{u}\right)}{\partial t}+\left(\nabla\cdot\varepsilon\rho_g\mathbf{u}\mathbf{u}\right)=-\varepsilon\nabla p+\mathbf{S}_p-\nabla\cdot\left(\varepsilon\boldsymbol{\tau}\right)+\varepsilon\rho_g\mathbf{g} \tag{2}$$

where ε is the porosity, ρ_g, $\mathbf{u}$, $\boldsymbol{\tau}$ and p respectively the density, velocity, viscous stress tensor, and pressure of the gas phase. The source term $\mathbf{S}_p$ is a function of the drag coefficient β, the details of which can be found in reference (6). To calculate the drag coefficient, we employ the well-known Ergun equation (10) for porosities lower than 0.8 and Wen and Yu correlation (11) for porosities higher than 0.8.

The equation of motion for an arbitrary particle, a, follow from Newton's second law

$$m_a\frac{d^2\mathbf{r}}{dt^2}=\mathbf{F}_{cont,a}+\mathbf{F}_{vdw,a}+\frac{V_a\beta}{1-\varepsilon}\left(\mathbf{u}-\mathbf{v}_a\right)-V_a\nabla p+m_a\mathbf{g}\,,\quad I_a\frac{d^2\boldsymbol{\theta}}{dt^2}=\mathbf{T}_a \tag{3}$$

where m_a is the mass of the particle, $\mathbf{F}_{cont,a}$ the contact force, $\mathbf{F}_{vdw,a}$ the van der Waals force, $\mathbf{T}_a$ the torque, I_a the moment of inertia, and $\boldsymbol{\theta}$ the angular displacement. These equations are solved numerically using a standard first-order time-integration scheme.

Contact forces

The contact forces between two particles (or between a particle and a wall) are calculated from the soft-sphere model developed by Cundall and Strack (12). In that model, a linear spring and a dashpot are used to compute the normal contact force, while a linear spring, a dashpot and a slider are used to compute the

tangential contact force (where the tangential spring stiffness is two seventh of the normal spring stiffness) ([13]). The tangential contact force can, in principle, be derived from a Coulomb-type friction law. However, we employ restitution coefficients rather than the damping coefficients. The relationship between these two coefficients can be found in ([13]).

Interparticle van der Waals forces

To calculate the interparticle van der Waals forces, we adopt the Hamaker relation ([14]),

$$F_{vw} = -\frac{A}{3} \frac{2r_1 r_2 \left(S + r_1 + r_2\right)}{\left[S\left(S + 2r_1 + 2r_2\right)\right]^2} \left[\frac{S\left(S + 2r_1 + 2r_2\right)}{\left(S + 2r_1 + 2r_2\right)^2 - \left(r_1 - r_2\right)^2} - 1\right]^2 \tag{4}$$

where S is the intersurface distance between two spheres, r_1 and r_2 the radii of the two spheres respectively. A is the Hamaker constant, which depends on the material properties. Note that Eq.4 exhibits an apparent numerical singularity, that is, the van der Waals interaction diverges if the distance between two particles approaches zero. In reality such a situation will never occur, because of the short-range repulsion between particles. In the present model, we have not included such a repulsion, since we can avoid the numerical singularity by defining a cut-off (maximal) value of the van der Waals force between two spheres. In practice, however, it is more convenient to use a cut-off value for the intersurface distance, S_0 ([15]).

SIMULATIONS RESULTS AND DISSCUSION

The effect of particle-particle contact parameters

Since in the homogeneous fluidization regime particle-particle contacts (or particle-particle collisions) occur frequently, a good understanding of their effect on the homogeneous fluidization is essential. The particle-particle contact is typically a dissipative process in which the kinetic energy of particles will be lost. In the soft-sphere model, two parameters will control the energy dissipation: the restitution coefficient and the friction coefficient. Simulations have been carried out for different restitution coefficients and friction coefficients (see Figure (1) for some typical snapshots). All the simulations have been performed under similar conditions, except for the values of the restitution and friction coefficients. It can be seen that in the absence of friction the cavities and channels are only found near the bottom of the bed, and furthermore wave-like surface is observed. If a non-zero friction coefficient is employed, we find the phenomena similar to those observed by Massimilla et al. ([16]): the channels form near the bottom of the bed and rise, grow and eventually disappear at the surface of the bed. Note that the surface of the bed is more flat in the presence of friction.

It may be deduced from the simulation results that the friction coefficient is the dominant parameters that affects the formation of channels and not the restitution coefficients. From granular physics, it is well-known that the kinetic energy dissipation between particle-particle contacts (collisions) will lead to the formation of clusters, and hence void structures such as cavities. This dissipation

can be caused by two types of interactions: the inelastic collision between particles, which is controlled by the restitution coefficient, and friction, which can be taken into account via the friction coefficient.

From the viewpoint of energy balance, the homogeneous fluidization regime can be considered as a quasi-equilibrium state. Due to the lack of bubbles that carry out the excess gas, the energy balance can be written as

$$E_i = E_o + E_d + E_p \tag{5}$$

where E_i is the kinetic energy provided by the inlet gas flow, E_o the kinetic energy carried out by the outlet gas flow, E_d the energy dissipated from particle-particle contacts, and E_p the potential energy necessary for maintaining the bed height. Interestingly, it is found from the simulation results that the average bed height will not change by modifying the contact parameters, as long as the inlet gas velocity is kept constant. Therefore the energy balance will be greatly affected by the dissipation of kinetic energy of particles due to particle-particle collisions. The presence of friction, on the other hand, may enhance the energy dissipation caused by particle-particle collisions. The wave-like surface of the bed in the absence of friction may relate to the energy distribution. We argue that in the absence of friction, the restitution coefficients in our simulations are not sufficient to keep the energy balance between E_i and E_d, and the gas motion may manifest in other complex forms. This suggests that the contact parameters, especially the frictional coefficients, will influence the energy distribution and hence hydrodynamics of the fluidized bed.
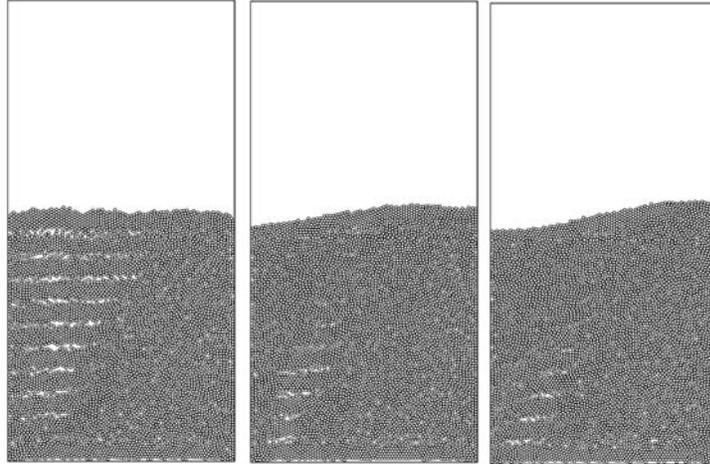

Figure 1: Snapshots obtained from simulations with different contact parameters. 6000 particles with a uniform size of 60 μm and a density of 1129 kg/m^3 are used. The normal and tangential spring stiffness are 7 N/m and 2 N/m respectively. The contact parameters in the pictures from left to right are: left: $e_n=e_t=0.9$, $\mu_f=0.3$; middle: $e_n=e_t=0.6$, $\mu_f=0.0$; right: $e_n=e_t=0.9$, $\mu_f=0.0$. The Hamaker constant is $A = 1.0\times10^{-20}$ J.

The forces structure during homogeneous fluidization

The effects of the interparticle van der Waals forces on the flow patterns inside fluidized beds have been reported in a previous paper ([9]). It was shown that in the case of strong van der Waals forces Geldart A particles manifest a Geldart C type behavior. In case of relatively weak interparticle van der Waals forces, we observed a fluidization behavior with some of the typical features found in fluidization experiments with Geldart A particles; for example, we observed the homogenous expansion, the gross circulation in the absence of bubbles and the presence of fast bubbles.

Here we will present a more detailed analysis of the magnitude of the various forces in the homogeneous fluidization regime. From Eq.3, we have the following total force (F_t), acting on a single particle

$$F_t = F_{cont,c} + F_{cont,f} + F_{vdw} + F_{drag} + F_g \qquad (6)$$

with $F_{cont,c}$ the elastic force due to particle-particle contact, $F_{cont,f}$ the friction
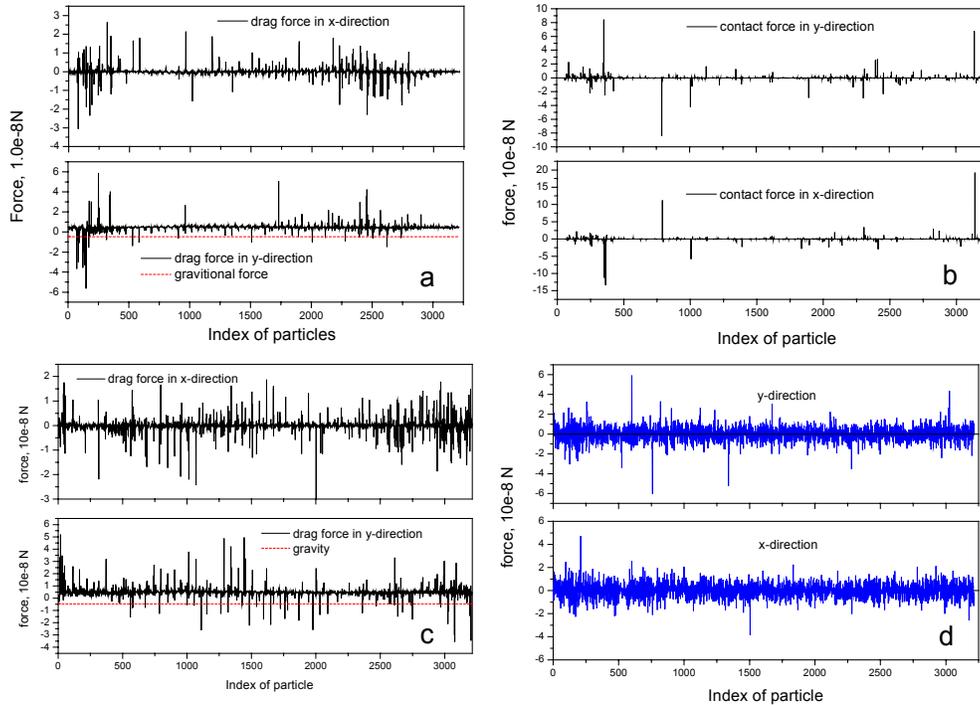

Figure 2: Forces acting on the particles during the homogeneous fluidization regime for different values of the Hamaker constant *A*. It is taken from one typical instant of the simulation, which is carried out with 3214 particles with a uniform size of 100 μm and a density of 900 kg/m^3. The normal and tangential spring stiffness are 7 N/m and 2 N/m, respectively. The contact parameters are: e_n=e_t=0.9, μ_f=0.2. (a) Drag force and gravitational force for *A* = 0; (b) Normal contact force for *A* = 0; (c) Drag force and gravitational force for *A* = 1.0×10^{-20}J; (d) The sum of van der Waals force and normal contact force for *A* = 1.0×10^{-20} J.

force due to particle-particle contact, F_{vdw} the van der Waals force, F_{drag} the drag force, and F_g the gravitational force. Simulations have been carried out both with and without interparticle van der Waals forces. In a recent paper ([17]) it was shown that the contact force acting on the particle will be balanced by the interparticle van der Waals forces. In Figure 2 we show the forces acting on each particle. In the presence of van der Waals forces it can be seen that the sum of normal contact force and interparticle van der Waals force is not strictly zero for most of particles, but rather fluctuates around zero. If we turn off the interparticle van der Waals force the normal contact force becomes extremely small (for most of particles it vanishes). Meanwhile, in both situations the x-components of the drag forces acting on the particles also fluctuate around zero while the y-components fluctuate around $-F_g$. The frictional forces between particles, however, are not balanced by any kinds of forces. Since the frictional forces are essentially working along the tangential direction, they may contribute much more to the rotational motion rather than the translational motion. Clearly, an exact balance of the forces seems to exist only at the macroscopic-level, but not at the level of individual particles, which confirms that the homogeneous fluidization regime is actually a quasi-equilibrium state. The drag forces and van der Waals forces are two important sources of the local force fluctuations, which consequently form the sources of velocity fluctuation of particles.
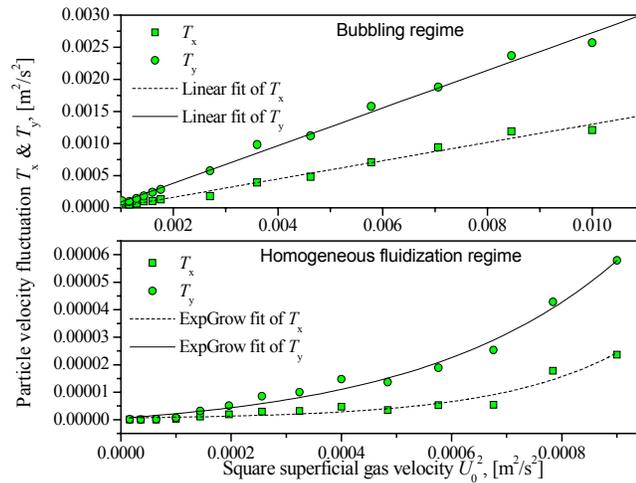
Velocity fluctuation of particles

Figure 3: The dependence of the velocity fluctuation of particles on the square superficial gas velocity. Simulations are carried out under the same conditions as indicated in Figure 2 except that the contact parameters are: $e_n=e_t=0.9$, $\mu_f=0.2$ and the Hamaker constant A = 1.0×10^{-20} J.

Due to the apparent difficulty of direct measurement of the velocity fluctuation of particles (i.e. granular temperature) in a gas-fluidized bed, only very recently some experimental results have become available. Cody et al. ([1]) measured the granular temperature in a gas-fluidized bed by use of a Acoustic Shot Noise (ASN) method. Menon and Durian ([18]) measured the sand motion in a gas-

fluidized bed with a diffusing wave spectroscopy (DWS). In a recent experiment ([19]) the fluctuation velocity $v = \sqrt{T}$ was estimated from the measured diffusion coefficient D_f by use of the kinetic theory. The velocity fluctuation of particles, with respect to the squared superficial gas velocity, obtained in our 2D simulations is plotted in Figure 3, It shows that the velocity fluctuation of particles is essentially zero before the bed begins to bubble, in agreement with the observation of Cody et al. ([1]) and Menon and Durian ([18]). Menon and Durian concluded that the homogeneous fluidization is a completely static state. Actually the velocity fluctuation of particles in the homogeneous fluidization regime is quite low (only 1% of that in bubbling regime), as shown in Figure 3, which is quite difficult to be measured by using a single measuring system due to the limited range of resolution. In this respect, the discrete particle simulations are ideally suited for obtaining this type of information.

Cody et al. ([1]) found that beyond the minimum fluidization point the average velocity fluctuation of particles is a linear function of the squared superficial gas velocity. It can be seen that in bubbling regime our simulation results agree very well with the findings by Cody et al. ([1]). In the homogeneous fluidization regime, however, we do not observe such a linear dependence, instead, we find an exponential dependence. It is noteworthy that in the experiments by Valverde et al. ([19]) an exponential dependence of the fluctuation velocity on gas velocity was found up to a maximum value corresponding to the maximum bed expansion point. In fact the interval of homogeneous fluidization in the experiments of Cody et al. ([1]) is quite short ($u_{mb}/u_{mf} < 2.0$, where both u_{mb} and u_{mf} have their normal meaning) and the exponential dependence of velocity fluctuation may be screened by the relatively long interval of the bubbling regime. In contrast, Valverde et al. ([19]) obtained a long interval of homogeneous fluidization ($u_{mb}/u_{mf} \approx 40$) by adding flow conditioners to particles with average diameter of 8.53 μm, where the cohesion of particles has been greatly reduced and a Geldart A type fluidization behavior is observed. So far the constant ratio of T_x / T_y in bubbling regime, as found in our previous simulation results ([9]), is actually due to the linear dependence of the velocity fluctuation of particles on the square superficial gas velocity.

The mechanism behind the transition from an exponential dependence to a linear dependence may be explained from the viewpoint of energy balance. The linear dependence may indicate that the fluctuation energy in the bubbling regime mainly comes from the energy provided by the inlet gas, while an exponential dependence hints at a more complicated picture. This will be the subject of further study.

CONCLUSIONS

By use of a soft-sphere discrete particle model, we investigated the homogeneous fluidization behavior of Geldart A particles in this paper. First the effect of contact parameters on the simulation of homogeneous fluidization of Geldart A particles is discussed. It is found that the particle-particle contact parameters will influence the energy distribution and consequently the hydrodynamics of the dense gas-solid flows in the fluidized bed. The formation of cavities and channels is related to the contact parameters, especially the friction coefficient. The structure of the forces acting on the particles is also studied, and the homogeneous fluidization

regime is shown to be a quasi-equilibrium state where a force balance only exists at the macroscopic-level but not at the level of individual particles. The drag forces and van der Waals forces are two important sources of the local force fluctuations, which consequently form the sources of velocity fluctuation of particles. Further analysis suggests that the velocity fluctuation of the particles is an exponential function of the squared superficial gas velocity in the homogeneous fluidization regime, and not a linear function as found by Cody et al. (1). So far the homogeneous fluidization is shown to represent a quasi-equilibrium phase resulting from a competition of three kinds of basic interactions: the fluid-particle interaction, the particle-particle collisions (and particle-wall collisions) and the interparticle van der Waals forces.

ACKNOWLEDGMENT

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