Hydrodynamic modeling of particle rotation for segregation in bubbling gas-fluidized beds

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Abstract

A multi-fluid Eulerian model has been improved by incorporating particle rotation using kinetic theory for rapid granular flow of slightly frictional spheres. A simplified model was implemented without changing the current kinetic theory framework by introducing an effective coefficient of restitution to account for additional energy dissipation due to frictional collisions. Simulations without and with particle rotation were performed to study the bubble dynamics and bed expansion in a monodispersed bubbling gas-fluidized bed and the segregation phenomena in a bidispersed bubbling gas-fluidized bed. Results were compared between simulations without and with particle rotation and with corresponding experimental results. It was found that the multi-fluid model with particle rotation better captures the bubble dynamics and time-averaged bed behavior. The model predictions of segregation percentages agreed with experimental data in the fluidization regime where kinetic theory is valid to describe segregation and mixing.

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1. Introduction

It is not uncommon to encounter industrial applications of dense gas–solid-fluidized beds for mixtures of particles with different physical properties such as size and density. Examples of industrial applications are coal gasification, fluidized bed polymerization and granulation. In such systems, the mixing of solids is often incomplete and a vertically non-uniform blend of particles forms. For example, in a system consisting of particles of equal density but different sizes, the bigger particles tend to reside at the bottom of the bed if the inlet velocity does not exceed the minimum fluidization velocity of the bigger particles. The bigger particles in this case are commonly referred to as jetsam. Smaller particles will float and reside at the top of the bed, commonly referred to as floatsam (Hoffmann et al., 1993). Knowledge of the degree and rate of this kind of segregation phenomena is very important for several reasons. In many industrial-fluidized beds, good mixing is required for uniform product quality or to avoid defluidization. In other applications, however, the tendency for segregation is utilized such as the case for continuous removal of a product.

Segregation phenomena in gas-fluidized beds have been extensively studied. Hoffmann et al. (1993) experimentally studied systems consisting of particles of equal density but different sizes. Wu and Baeyens (1998) also examined the behavior of equal density systems of large and small particles. They showed segregation patterns where larger particles migrated to the bottom, whereas the smaller particles concentrated at the top section of the bed. Nienow and Naimer (1980) performed experiments on systems consisting of particles of equal size but different density. These studies indicate that mixing and segregation of bubbling-fluidized beds are largely determined by the bubble dynamics. Bubbles act as a vehicle for both mixing and segregation. Goldschmidt et al. (2003) measured bed expansion and segregation dynamics with particles of well-known properties (size, shape, density and collision properties) in dense gas-fluidized bed using digital image analysis. An advantage of the experimental setup is that it can be easily simulated numerically using robust hydrodynamic models.
Numerical simulations of the hydrodynamics of gas-fluidized beds have been employed as a useful tool to study segregation phenomena. Recently, Hoomans et al. (2000) showed bubble dynamics in dense gas-fluidized beds strongly depend on the amount of energy dissipated by particle–particle collisions using hard sphere discrete particle models. (Goldschmidt et al., 2001a,b; Goldschmidt, 2001) used Eulerian models to study the segregation phenomena in bubbling gas-fluidized beds. The number of particles specified using a discrete particle model (typically less than $10^6$) was an order of magnitude lower than that encountered in most industrial-fluidized beds (Goldschmidt, 2001).

In order to describe the segregation phenomena in large industrial-scale-fluidized bed reactors, a multi-fluid Eulerian model is better than a Lagrangian model due to the computational expense to simulate large numbers of particles. In this kind of model both gas and particulate phases are described as interpenetrating continua and the kinetic theory of granular flow (KTGF) is used to provide constitutive closures for particulate phases. Although Eulerian models have been developed and used to study bed hydrodynamics and segregation (Goldschmidt et al., 2001a,b; Goldschmidt, 2001; Enwald et al., 1996; Gidaspow, 1994), these models cannot describe quantitatively segregation rates in polydisperse-fluidized beds. For example, higher segregation rates were predicted by numerical simulations compared with experiments, as reported by Goldschmidt et al. (2001b). It is speculated that KTGF, which is limited to slightly inelastic spherical particles and does not allow for particle rotation, underestimates the amount of energy dissipated in the frictional inelastic collisions for common particles. Consequently, the bubble intensity is underestimated. Further studies (Goldschmidt, 2001) showed that the absence of rotation and subsequent energy losses is a deficiency of the multi-fluid model in contrast to discrete particle models which provide closer resemblance to experimental results. Therefore, it should be of interest to incorporate particle rotation into the hydrodynamic model and analyze the effects on segregation in gas-fluidized beds.

In principle, particle rotation can be incorporated in a multi-fluid model by addition of conservation equations for angular momentum and rotational granular temperature. Jenkins and Richman (1985) and Lun and Savage (1987) derived models for rough disks and spheres, respectively. The kinetic energies associated with fluctuations in both translational velocity and spin were considered. The additional equations for angular momentum and rotational granular energy greatly increase the complexity of the kinetic theory. Since the most important influence of particle rotation on bed dynamics is the energy dissipation, a simpler approach which only modifies the granular energy dissipation seems promising.

In this work, particle rotation is incorporated into a multi-fluid Eulerian model using a simple kinetic theory for rapid granular flow of slightly frictional spheres (Jenkins and Zhang, 2002). The improved multi-fluid Eulerian model is used to study the size-driven segregation in a bidispersed gas–solid-fluidized bed. Results from the particle rotation model are compared with numerical simulations without particle rotation and with corresponding experimental results.

2. Methodology

2.1. Basic multi-fluid model

A Fortran code, Multiphase Flow with Interphase eXchanges (MFIX), is used for all simulations in this work. The multi-fluid Eulerian model in MFIX divides the particle mixture into a discrete number of phases, each of which can have different physical properties and can be mathematically described as interpenetrating continua. The governing equations for the multi-fluid model are as follows (Syamlal et al., 1993):

Continuity equation for gas phase

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{V}_g) = \sum_{n=1}^{N_g} \mathbf{R}_{gn}. \tag{1}$$

Continuity equation for $m$th solid phase

$$\frac{\partial}{\partial t}(\varepsilon_{sm} \rho_{sm}) + \nabla \cdot (\varepsilon_{sm} \rho_{sm} \mathbf{V}_{sm}) = \sum_{n=1}^{N_{sm}} \mathbf{R}_{smn}. \tag{2}$$

Momentum equation for gas phase

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \mathbf{V}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{V}_g \mathbf{V}_g) = \nabla \cdot \mathbf{S}_g + \varepsilon_g \rho_g \mathbf{g} - \sum_{m=1}^{M} \mathbf{T}_{gm}. \tag{3}$$

Momentum equation for $m$th solid phase

$$\frac{\partial}{\partial t}(\varepsilon_{sm} \rho_{sm} \mathbf{V}_{sm}) + \nabla \cdot (\varepsilon_{sm} \rho_{sm} \mathbf{V}_{sm} \mathbf{V}_{sm}) = \nabla \cdot \mathbf{S}_{sm} + \varepsilon_{sm} \rho_{sm} \mathbf{m} + \mathbf{T}_{gm} - \sum_{i=1, l \neq m}^{M} \mathbf{T}_{im}. \tag{4}$$

Translational granular temperature equation (Agrawal et al., 2001)

$$\frac{3}{2} \left[ \frac{\partial}{\partial t} \varepsilon_{sm} \rho_{sm} \theta_{sm,t} \right] + \nabla \cdot (\varepsilon_{sm} \rho_{sm} \theta_{sm,t} \mathbf{V}_{sm}) = \nabla \cdot \mathbf{S}_{sm} - \mathbf{S}_{sm} \cdot \nabla \mathbf{V}_{sm} + \gamma_{sm,slip} - J_{sm, coll} - J_{sm, vis}, \tag{5}$$

where the translational granular temperature is defined as

$$\theta_{sm,t} = \frac{1}{3} \langle C_{sm}^2 \rangle. \tag{6}$$

The fluctuation in the particle translational velocity shown in Eq. (6) is defined as $\mathbf{C}_{sm} = \mathbf{c}_{sm} - \langle \mathbf{c}_{sm} \rangle$, where $\mathbf{c}_{sm}$ is the instantaneous translational velocity and $\langle \mathbf{c}_{sm} \rangle$ is the ensemble average.

Constitutive equations for the gas phase stress tensor ($\mathbf{S}_g$) and gas–solid momentum transfer ($\mathbf{I}_{sm}$) can be found in Syamlal et al. (1993). The solid–solid interaction term ($\mathbf{I}_{sm}$) was derived by Syamlal (1987) using a simple model from
kinetic theory, in which singlet velocity distribution functions were expressed as Dirac delta functions. Thus, granular temperature terms do not appear in the solid–solid interaction. The constitutive equations for multi-component solid mixtures are derived from granular flow theory. There are two distinct flow regimes for granular flow: a viscous or rapidly shearing regime in which stresses arise due to collisional or translational momentum transfer, and a plastic or slowly shearing regime in which stresses arise due to Coulomb friction between particles in enduring contact (Syamlal et al., 1993). The rapid granular flow regime is of main interest in this research. The constitutive equations used in MFIX for this regime were derived based on kinetic theory of granular flow, derived by Lun et al. (1984) and modified by Ma and Ahmadi (1988) to take into account the effects of interstitial gas on particle phase viscosity and thermal diffusivity.

The constitutive relationship and boundary conditions, which will be modified in the particle rotation model, are shown in the following. The rate of dissipation of translational fluctuation kinetic energy due to particle collisions is defined as

$$J_{\text{sm,coll}} = \frac{12}{\sqrt{\pi}} (1 - e_{\text{sm}}^2) \rho_{\text{sm}} \frac{e_{\text{sm}}}{dm} g_{\text{nm}} \theta_{\text{sm,t}}^{3/2}. \quad (7)$$

The partial slip boundary conditions for particle–wall interactions, proposed by Johnson and Jackson (1987), are employed. The boundary condition for the slip velocity is

$$\vec{V}_{\text{sm,slip}} \cdot \vec{S}_{\text{sm}} \cdot \vec{n} + \frac{\sqrt{3}}{6} \phi \rho_{\text{sm}} g_{\text{nm}} \theta_{\text{sm,t}}^{1/2} |\vec{V}_{\text{sm,slip}}| = 0. \quad (8)$$

The boundary condition for the flux of translational fluctuation energy to the wall is

$$-\vec{n} \cdot \vec{q}_{\text{sm}} = \frac{\sqrt{3}}{4} \pi (1 - e_{\text{sm}}^2) e_{\text{sm}} \rho_{\text{sm}} g_{\text{nm}} \theta_{\text{sm,t}}^{3/2} + \vec{V}_{\text{sm,slip}} \cdot \vec{S}_{\text{sm}} \cdot \vec{n}, \quad (9)$$

where

$$\vec{V}_{\text{sm,slip}} = \vec{V}_{\text{sm}} - \vec{V}_w. \quad (10)$$

2.2. Particle rotation model

Most common particles are frictional as well as inelastic. As a result, particles can rotate with angular velocity $\vec{\omega}$ and translate under rapid rates of deformation. Lun et al. (Lun and Savage, 1987; Lun, 1991) developed a kinetic theory for a system of inelastic, rough surfaces to study the effects of particle surface friction and rotational inertia. Jenkins and Richman (1985) used Grad’s method of moments to derive conservation laws and constitutive relations for planar flows of a dense gas consisting of identical, rough, inelastic, circular disks. In these theories (Lun and Savage, 1987; Lun, 1991; Jenkins and Richman, 1985), two granular temperatures are involved. The first is translational granular temperature $\theta_t$, which measures the energy associated with the translational velocity fluctuations, as defined in Eq. (6). The second is rotational granular temperature $\theta_r$, which measures the energy associated with the angular velocity fluctuations, defined as $\theta_r = \langle (1/3 m_p) I \dot{\Theta}^2 \rangle$, where $I$ is moment of inertia, $\dot{\Theta} = \dot{\Theta} - \langle \dot{\Theta} \rangle$ is the angular velocity fluctuation and $m_p$ is the mass of a particle. Additional conservation equations for angular momentum and rotational granular temperature are required, which greatly increase the complexity of the kinetic theory and is often difficult to apply to general flows. Since the most important influence of particle rotation on bed dynamics is the additional energy dissipation due to frictional collisions, a simpler approach which only modifies the translational granular energy seems promising.

A simple model from kinetic theory for rapid flow of identical, slightly frictional, nearly elastic spheres (Jenkins and Zhang, 2002) was adapted to incorporate particle rotation into the multi-fluid model presented in the previous section. In this model, the frictional collision is described by a normal restitution coefficient $e$, a friction coefficient $\mu$ and a tangential restitution coefficient $\mu_0$. For slightly frictional spheres, the distribution of translational velocities does not differ too much from that for smooth spheres. The balance equations for the moments associated with the rotational degree of freedom are satisfied in an approximate way by ignoring unsteady and inhomogeneous terms. Thus, the conservation of angular momentum reduces to the requirement that the mean spin of spheres be equal to half the vorticity of their mean velocity. The conservation of rotational granular energy is approximately satisfied by requiring that the net rate of energy production for the angular velocity fluctuations is zero. The influence of friction on the collisional transfer of linear momentum and translational energy is negligible, and the stress and the translational energy flux are identical to those for smooth, elastic spheres. Only the dissipation rates for translational and rotational granular energy, $J_{\text{sm,coll}}$ and $\Gamma_{\text{sm}}$, respectively, are influenced by friction. The approximations of $J_{\text{sm,coll}}$ and $\Gamma_{\text{sm}}$ are (Jenkins and Zhang, 2002):

$$J_{\text{sm,coll}} = \frac{12}{\sqrt{\pi}} \rho_{\text{sm}} \frac{e_{\text{sm}}^2}{dm} g_{\text{nm}} \theta_{\text{sm,t}}^{3/2} \times \left[ 2(1 - e_{\text{sm}}) + a_1 - a_2 \frac{\theta_{\text{sm,r}}}{\theta_{\text{sm,t}}} \right], \quad (11)$$

where

$$a_1 = \frac{\mu}{\mu_0} \left[ \pi \mu_0 \left( 1 - \frac{2}{\pi} \arctan \mu_0 \right) + \frac{2 \mu_0^2}{1 + \mu_0} \left( 1 - 2 \frac{\mu}{\mu_0} \right) \right], \quad (12)$$

$$a_2 = \frac{5 \mu}{\mu_0} \left[ \frac{\pi}{2} \mu_0 \left( 1 - \frac{2}{\pi} \arctan \mu_0 \right) - \frac{\mu_0^4}{(1 + \mu_0^2)^2} \right], \quad (13)$$

and

$$\Gamma_{\text{sm}} = -\frac{120}{\sqrt{\pi}} \frac{\rho_{\text{sm}}^2}{d_{\text{pm}}} g_{\text{nm}} \theta_{\text{sm,t}}^{3/2} \left[ b_1 - b_2 \frac{\theta_{\text{sm,r}}}{\theta_{\text{sm,t}}} \right], \quad (14)$$
Thus, the kinetic theory for slightly frictional, nearly elastic and the partial slip boundary condition for the flux of cation to the multi-fluid model is through the introduction of translational temperature need to be considered. The modification to the multi-fluid model is through the introduction of an effective coefficient of restitution that incorporates the additional dissipation due to frictional interactions in the rate of dissipation of translational fluctuation energy.

Substituting Eq. (18) to Eq. (11) and comparing the result to Eq. (7), we can define an effective coefficient of restitution (assuming that \(1 + \varepsilon_{sm}\) \(\approx 2\), i.e., nearly elastic):

\[
\varepsilon_{sm, eff} = \frac{1}{2} a_1 + \frac{a_2 b_1}{2 b_2}.
\]

Thus, the kinetic theory for slightly frictional, nearly elastic spheres has the same structure as that for frictionless spheres, i.e., only conservation of mass, mean translational velocity and translational temperature relative to the height and width (see Table 1). The thin depth suppresses particle motion in that direction in the experiments and the effect of the front and back walls to the bed was not considered of interest (Goldschmidt, 2001).

A two-dimensional computational domain was used in the fluidized bed simulations, which is a physical reliable model of the pseudo-two-dimensional experiment. The dimensions are shown in Fig. 1 for a Cartesian coordinate system. The domain and grid size are specified in Table 2. Although the experiment used a system with a domain height of 70 cm, the computational domain height was reduced to 45 cm to avoid computationally expensive simulations yet ensuring the bed dynamics are physical. It was evident from the experiments that the bed did not expand above 30 cm. The particle properties and collision parameters cited in the experiments (see Table 1) are used as input parameters for the numerical work to test and validate the particle rotation model. The effective coefficients of restitution for these two kinds of particles are calculated using Eq. (19) and the values are shown in Table 1.

A spatial grid refinement study was performed to determine the grid sensitivity of the computational results. Three successively halved grids, i.e., coarse, medium and fine grids, were

### Table 1

| Geometry of the experimental system and particle properties (Goldschmidt, 2001) |
|---|---|---|
| Height | 70 cm |
| Width | 15 cm |
| Depth | 1.5 cm |

| Particle–particle collision parameters |
|---|---|---|
| \(\varepsilon_{sm} \) | 0.97 \(\pm\) 0.01 | 0.97 \(\pm\) 0.01 |
| \(\mu \) | 0.15 \(\pm\) 0.015 | 0.10 \(\pm\) 0.01 |
| \(\beta_0 \) | 0.33 \(\pm\) 0.05 | 0.33 \(\pm\) 0.05 |
| \(\varepsilon_{sm, eff} \) | 0.83 | 0.86 |

| Particle–wall collision parameters |
|---|---|---|
| \(\varepsilon_w \) | 0.97 \(\pm\) 0.01 | 0.97 \(\pm\) 0.01 |
| \(\mu_w \) | 0.10 \(\pm\) 0.015 | 0.09 \(\pm\) 0.01 |
| \(\beta_0, w \) | 0.33 \(\pm\) 0.05 | 0.33 \(\pm\) 0.05 |
| \(\varepsilon_{w, eff} \) | 0.86 | 0.87 |
used. The study showed that the grid refinement from coarse to medium grid size improved the results by a relatively large degree, while refinement from medium to fine grid size had little influence on time-averaged results. A Richardson extrapolation based on the medium and fine grids was used to provide error estimates. The time-averaged voidage for medium grid had an average error of 1.4% and a maximum error of 3.7%, compared to the Richardson extrapolation results. As a conclusion from the grid refinement study, the medium grid size was used for the remaining simulations as given in Table 2. In addition, the current grid size is of the order of a few particle diameters, which is thought to adequately resolve the meso-scale structures of gas–solid flows (Agrawal et al., 2001). Computational results were not sensitive to time step change since an adaptive time stepping algorithm was used. For all simulations, the initial and boundary conditions are listed in Table 2, and numbers for the minimum fluidization voidage and inlet gas velocity will follow in the text.

A case simulating the monodispersed powder of large particles was first performed to calibrate the particle rotation model incorporated into MFIX. The minimum fluidization voidage \( \varepsilon_{mf} \) was set to 0.417 and the gas inflow velocity was 1.5 \( U_{mf} \), where the \( U_{mf} \) is for large particles (see Table 1). Simulations without and with particle rotation were run for 10 s. The instantaneous gas volume fractions are shown at 2-s intervals in Fig. 2. Each subfigure (a–f) has a pair of frames, whereby the left frame shows results for the simulation without particle rotation and the right frame shows results with particle rotation. The model with particle rotation predicts bigger bubbles and higher gas volume fractions compared to the model without particle rotation. The primary reason is that more energy dissipates due to particle rotation and particle velocities decrease after impact, leading to a more closely spaced particle ensemble and thus higher gas volume fraction. A consequence is that gas–solid interactions exert higher drag forces on particles and cause the particles to move vigorously. Thus, particle rotation increases the bubble intensity, which is consistent with the numerical findings of Hoomans et al. (1996) using a discrete particle model.

Time-averaged results were analyzed after 5 s to avoid initial transient fluctuations. Averaging from 5 to 10 s is sufficient since further averaging in time beyond 10 s provides no new additional information for this monodispersed system. The solid volume fraction averaged over 5–10 s is shown in Fig. 3 (a) and (b) without and with particle rotation, respectively. The particle volume fraction profile without particle rotation has a more homogeneous distribution. With particle rotation, higher particle volume fractions were obtained near the walls and larger bubbles formed in the bed center as was demonstrated in Fig. 2. This near-wall distribution is consistent with experimental observations of Goldschmidt (2001). In Fig. 4, a similar comparison shows that the particle rotation model also predicts better particle distribution for the same case where the inlet gas velocity is increased to 2.0 \( U_{mf} \).

To characterize the bed expansion, an average particle height is defined as

\[
\langle h_p \rangle = \frac{\sum_{i} N_{part} \bar{h}_i}{N_{part}} = \frac{\sum_{k} N_{cells} \varepsilon_{s,k} \bar{h}_k}{\sum_{k} N_{cells} \varepsilon_{s,k}}. \tag{22}
\]

The time-averaged particle height was calculated over 5–10 s. The \( \langle h_p \rangle \) from the simulations without and with particle rotation.
rotation were compared with the experimental data in Table 3. Overall, the model with particle rotation was able to better capture bubble dynamics and bed expansion of monodispersed gas–solid-fluidized systems. Based on these results for a monodispersed-fluidized bed, the particle rotation model should better predict the segregation phenomena in a polydispersed system where bubbles play a dominant role in transporting particles.

Simulations of a binary mixture of small and large particles were examined next. The minimum fluidization voidage is also 0.417. The initial gas velocity \( V_g \) was set as the minimum fluidization velocity of the small particles in the freeboard region. The mass fraction of the small particles \( x_{\text{small}} \) was 0.5. Small and large particles were perfectly mixed. This assumption yields equal volume fractions of both small and large particles assuming that the maximum packing density in a fluidized state for small and large particles are equal. The gas inflow velocity is 1.3 m/s, slightly higher than the minimum fluidization velocity of the larger particles. Simulations without and with particle rotation were both run for 20 s each.

Fig. 5 shows bubble dynamics of the binary mixture system without and with particle rotation. The instantaneous gas volume fractions are shown in Fig. 5. Each subfigure (a–f) has a pair of frames, whereby the left frame shows results for the simulation without particle rotation and the right frame shows results for particle rotation. It can be seen that larger bubbles formed, i.e., the bubble intensity increased, with the inclusion of particle rotation.

To understand the particles distribution in the bed, time-averaged solid volume fractions spatially averaged over the bed width are shown in Fig. 6 with respect to the bed height. Each curve represents the particle distribution with respect to particle size and rotation. The model without particle rotation predicts significant segregation, whereby large particles predominately occupy the bottom of the bed and small particles reside closer to the top. In contrast, the solid volume fractions of the small and large particles based on the rotation model tend to be equally distributed throughout the bed. The model with particle rotation predicts better mixing except at the bottom, where there is a small difference between them. The model with particle rotation were both run for 20 s each.

Fig. 2. Instantaneous gas volume fraction for a monodispersed-fluidized bed with inlet gas velocity of 1.5 \( U_{mf} \) at (a) 0 s, (b) 2 s, (c) 4 s, (d) 6 s, (e) 8 s and (f) 10 s. For each subframe, the left side are simulations without particle rotation and the right frame with particle rotation.
Fig. 3. Time-averaged particle volume fraction for a monodispersed-fluidized bed with inlet gas velocity of 1.5 $U_{mf}$ for the model (a) without particle rotation and (b) with particle rotation.

rotation also predicts higher bed expansion because of larger bubble intensity as mentioned above.

To further investigate the segregation extent and rate, the segregation percentage is defined (Goldschmidt et al., 2003):

$$s_p = \frac{S_p - 1}{S_{p,\text{max}} - 1},$$

and $s_p$ equals 0 when the particles are perfectly mixed and 1 when the mixture has completely segregated. The parameter $S_p$ is the ratio of the average heights of the small and large particles according to Eq. (22):

$$S_p = \frac{\langle h_{\text{small}} \rangle}{\langle h_{\text{large}} \rangle}.$$  

The parameter $S_{p,\text{max}}$ is the maximum degree of segregation, which can be calculated in terms of mixture composition (assuming that the maximum packing density in the fluidized state for small particles equals that for large particles) from

$$S_{p,\text{max}} = \frac{2 - x_{\text{small}}}{1 - x_{\text{small}}}.$$  

Table 3

<table>
<thead>
<tr>
<th></th>
<th>1.5 $U_{mf}$ (m)</th>
<th>2.0 $U_{mf}$ (m)</th>
</tr>
</thead>
<tbody>
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<td>Experiments</td>
<td>0.1140</td>
<td>0.1180</td>
</tr>
<tr>
<td>Model without rotation</td>
<td>0.0921</td>
<td>0.1102</td>
</tr>
<tr>
<td>Model with rotation</td>
<td>0.0973</td>
<td>0.1176</td>
</tr>
</tbody>
</table>

Further simulations using MFIX (without and with the rotational model) were conducted for other bidispersed-fluidized bed systems (for example, the study by Hoomans et al., 2000). Results showed the same improvement: the rotational model effectively reduced segregation percentages as long as the inlet gas flow was within the same limits with respect to the small and large particle minimum fluidization velocities.

It is, however, worthwhile to point out that the particle rotation model does not have the same kind of improvement for segregation percentages and has a much higher segregation rate. The simulation with particle rotation, on the other hand, is in good agreement with the experimental data. For this case, recall that the inlet velocity was slightly greater than the minimum fluidization velocity for the larger particles. Thus, both small and large particles fluidize, creating a well-mixed system.

Fig. 4. Time-averaged particle volume fraction for a monodispersed-fluidized bed with inlet gas velocity of 2.0 $U_{mf}$ for the model (a) without particle rotation and (b) with particle rotation.

Fig. 7 shows the segregation percentage for the numerical simulations without and with particle rotation and how they compare to the experimental data provided by Goldschmidt (Goldschmidt et al., 2003; Goldschmidt, 2001). The experimental data were averaged over 1 s time intervals, while the numerical results are instantaneous values at 0.1 s time intervals. The simulation without particle rotation over-predicts the
segregation cases where the gas inlet velocity is between the minimum fluidization velocities of the small and large particles. As shown in Fig. 8, for a case with gas inlet velocity at 1.0 m/s, numerical results with and without particle rotation both predicted much higher segregation percentages than the experimental data. The particle rotation model predicted larger fluctuations of the segregation percentages, which can also be attributed to the increased bubble intensity by this model. The major discrepancy between numerical results and experimental results, however, is due to the fact that the large particles are not very well fluidized in this conditions and thus the “hindrance effect” (Gera et al., 2004) is produced between the small particles and the reluctant large particles. To account for this kind of hindrance effect is beyond the capability of the current kinetic theory for granular flows.

4. Conclusions

A multi-fluid Eulerian model has been improved by incorporating particle rotation using a simplified kinetic theory for rapid granular flow of slightly frictional spheres. Simulations without and with particle rotation were performed to study bubble dynamics in a monodispersed gas–solid-fluidized bed and segregation phenomena in a dense gas–solid-fluidized bed of a binary solid mixture. Results were compared between simulations with and without the particle rotation model and with corresponding experimental results. To the authors’ knowledge, this is the first time a multi-fluid model with particle rotation has been used to study segregation phenomena in gas-fluidized beds. In the monodispersed system, bubble intensity and bed expansion increased as a result of more energy dissipation with the particle rotation model, which better agrees with experimental results. In the binary systems studied in this paper, better agreement was achieved by using the model with particle rotation in the regime where kinetic theory is applicable and the particle–particle interactions have a noticeable effect on segregation. Despite these limitations on applications of the particle rotation model, preliminary results indicated that particle rotation is an important microscopic physics to be incorporated into the fundamental hydrodynamic model.

For further model development, the particle rotation effect can be more directly coupled to the momentum transfer between
solid phases, which is very important to segregation, in the following two aspects. First, the granular temperature can be included in the solids momentum transfer term. Second, the influence of particle rotation on collisional transfer of the linear momentum can be considered by more sophisticated kinetic theory. Whether including these two factors will better model segregation phenomena in bubbling gas-fluidized beds will be of interest for further investigation. The authors also recognize that the two-dimensional domain reduces the rotation effect, therefore, particle rotation in a three-dimensional domain will be addressed in future studies.

**Notation**

\[ \mathbf{\bar{c}} \]  
\[ \bar{C} \]  
\[ d \]  
\[ e \]  
\[ F \]  
\[ \mathbf{\bar{g}} \]  
\[ g_0 \]  
\[ I \]  
\[ \mathbf{\bar{I}} \]  
\[ J_{\text{coll}} \]  
\[ J_{\text{vis}} \]  
\[ m_p \]  
\[ \mathbf{\bar{n}} \]  
\[ R \]  
\[ \text{Re} \]  
\[ S_d \]  
\[ S_p \]  
\[ S \]  
\[ \bar{S} \]  
\[ U \]  
\[ \bar{V} \]  
\[ x \] 

instantaneous particle velocity  
translational particle velocity fluctuation  
particle diameter  
coefficient of normal restitution  
drag coefficient  
gravity  
equilibrium radial distribution function at contact  
moment of inertia of a particle  
interphase momentum transfer  
rates of dissipation of translational fluctuation kinetic energy due to particle collisions  
rates of dissipation of translational fluctuation kinetic energy due to interstitial gas viscous damping  
mass of a particle  
unit normal vector from a boundary to particles  
rates of formation  
Reynolds number  
segregation degree  
segregation percentage  
stress tensor  
velocity for gas and solids phases  
mass fraction
Greek letters

$\beta_0$ coefficient of tangential restitution

$\gamma_{\text{slip}}$ production of translational fluctuation kinetic energy due to gas–particle slip

$\Gamma$ rate of dissipation of rotational granular energy

$\theta_0$ rotational granular temperature

$\theta_1$ translational granular temperature

$\mu$ coefficient of friction

$\rho$ density

$\phi'$ specularity coefficient for wall

$\Phi$ particle shape factor

$\dot{\omega}$ particle angular velocity

$\bar{\Omega}$ fluctuation in particle angular velocity

Superscripts/subscripts

coll collision

eff effective parameters

g gas phase

$l$ $l$th solid phase

$m$ $m$th solid phase

max maximum value

$mf$ minimum fluidization

$M$ number of phases

$N$ number of species

$p$ particle

$r$ rotational

$s$ solid phase

$t$ translational

$w$ wall boundary

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