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Investigation of collisional parameters for rough spheres in fluidized beds

Lei Yang, J.T. (Johan) Padding *, J.A.M. (Hans) Kuipers

Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, 5600, MB, Eindhoven, The Netherlands

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ABSTRACT

The effect of normal restitution coefficient and friction coefficient on the hydrodynamics of a dense bubbling solid-gas fluidized bed is investigated using a two fluid model (TFM) based on our kinetic theory of granular flow (KTGF) for rotating frictional particles. A comparison between TFM simulations using the present KTGF model, and a simpler KTGF model for rapid flows of slightly frictional, nearly elastic spheres derived by Jenkins and Zhang [1], is carried out. The simulation results reveal that both the coefficient of normal restitution and friction coefficient play an important role in the homogeneity of the bubbling bed. The particle friction has a strong effect on the solids flow patterns and distribution, while the normal restitution coefficient has a relatively small effect on both. The present model also predicts a larger amount of energy dissipation caused by the inclusion of particle friction. The present KTGF model leads to better agreement with detailed discrete particle model (DPM) simulation results for the axial particle velocity profiles and solids volume fraction distribution.

1. Introduction

Gas-solid fluidized beds find a widespread application in processes involving combustion, separation, classification, and catalytic cracking [2]. Understanding the dynamics of fluidized beds is a key issue in improving efficiency, reliability and scale-up. Owning to enormous increase in computer power and algorithm development, fundamental modelling of multiphase reactors has become an effective tool.

In this work, an Euler-Euler approach (Kuipers et al. [3], Gidaspow [4]) is used. In Eulerian two fluid models (TFM), both the gas phase and the solid phase are treated as fully interpenetrating continua and are described by separate governing balance equations of mass and momentum. The challenge of this model is to establish an accurate hydrodynamic description of the solid phase. State-of-the-art closures have been obtained from the kinetic theory of granular flow (KTGF), initiated by Jenkins and Savage [5], Jenkins and Richman [6], Lun [7], and Nieuwland [8].

The original KTGF models of Jenkins and Savage [5], Jenkins and Richman [6] and Gidaspow [4] were derived for nearly elastic particles with translational motion only. In reality, however, granular materials are frictional. The roughness of the granular materials has been shown to have a significant effect on stresses at least in the quasi-static regime [9]. During collisions of rough particles, the particles can rotate due to the surface friction. Consequently, translational and rotational kinetic energies may exchange. Attempts to quantify the friction effect have been somewhat limited. Based on Lun and Savage [10], Walton [11] introduced coefficients of restitution associated with both the normal and tangential components of the velocity at the contact point. These coefficients can be measured by performing experiments with real particles [12–14]. Jenkins and Zhang [1] developed a simple kinetic theory for collisional flows of identical, slightly frictional, nearly elastic spheres. An effective restitution coefficient was given in terms of the collision parameters, namely the normal coefficient of restitution e, friction coefficient μ, and tangential coefficient of restitution β. This model is widely used in the study of the gas-solid fluidization [15–17]. Goldschmidt et al. [18] found that the effects of particle friction could not be replaced by using this effective (smaller) restitution coefficient. More recently, there have appeared some other works regarding the effect of particle friction. Van Wachem et al. [19] derived a simplified algebraic granular temperature equation. They found that this simplification does not lead to obvious differences in the simulation results, but reduces the computational time by about 20%. However, their model cannot be used for semi-dilute and dilute systems. The frictional kinetic model from Schneiderbauer et al. [20] is based the KTGF model from Agrawal et al. [21], which was originally developed for systems with mesoscale structures such as risers with particle clusters. This model includes closures for the solids stress tensor, which considers collisional, kinetic and frictional stress. However, as pointed out by themselves, this model lacks an explicit dependence on material properties of the particles. Berzi and Vescovi [22] found that the yield stress ratio of granular material can be theoretically predicted by the extended theory from Jenkins and Berzi [23], which reveals that the extended kinetic theory can obtain excellent agreement with numerical simulations on simple shearing of inelastic, frictional and frictionless particles. However, they also

* Corresponding author at: Process & Energy Department, Delft University of Technology, The Netherlands.
E-mail address: J.T.Padding@tudelft.nl (J.T.(J.) Padding).

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pointed out that the relation between the shear rigidity and the inter-particle friction is still lacking.

Yang et al. [24] developed a KTGF for rough spheres including particle friction and rotation, where the rheological properties of the solid phase are explicitly described in terms of the friction coefficient. This new model has been incorporated into our in-house two-fluid model (TFM) code for the modelling of dense gas-solid fluidized beds. This model has been validated for a bubbling fluidized bed by Yang et al. [25].

In this work, we employ the new KTGF model (called model A) and compare it with the effective model by Jenkins and Zhang (model B) to investigate the influence of friction coefficient and normal restitution coefficient on the properties of a gas-solid fluidized bed. Similar to previous studies in the literature [18,26], we will compare our results with detailed DPM simulation results, where DPM is used as an "independent" modelling framework to further validate our KTGF in TFM.

2. Numerical models

The two fluid model treats both phases as fully interpenetrating continua. The continuity equations for the gas and solid phases are given respectively by Eqs. (1) and (2). The corresponding momentum equations are given by Eqs. (3) and (4).

$$\frac{\partial\left(\varepsilon_g\rho_g\right)}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot\left(\varepsilon_g\rho_g\mathbf{v}_g\right)=0 \tag{1}$$

$$\frac{\partial(\varepsilon_s\rho_s)}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot(\varepsilon_s\rho_s\mathbf{v}_s)=0 \tag{2}$$

$$\begin{aligned}\frac{\partial\left(\varepsilon_g\rho_g\mathbf{v}_g\right)}{\partial t}+\nabla\cdot\left(\varepsilon_g\rho_g\mathbf{v}_g\mathbf{v}_g\right)=&-\varepsilon_g\nabla P_g-\nabla\cdot\varepsilon_g\boldsymbol{\tau}_g\\&+\varepsilon_g\rho_g\mathbf{g}-\beta_A\left(\mathbf{v}_g-\mathbf{v}_s\right)\end{aligned} \tag{3}$$

$$\begin{aligned}\frac{\partial(\varepsilon_s\rho_s\mathbf{v}_s)}{\partial t}+\nabla\cdot(\varepsilon_s\rho_s\mathbf{v}_s\mathbf{v}_s)=&-\nabla\cdot(P_s\mathbf{I}+\varepsilon_s\boldsymbol{\tau}_s)+\varepsilon_s\rho_s\mathbf{g}\\&+\beta_A\left(\mathbf{v}_g-\mathbf{v}_s\right)-\varepsilon_s\nabla P_g\end{aligned} \tag{4}$$

The gas and solid phases are coupled through the interphase momentum transfer coefficient β_A. To describe the solid phase, KTGF with friction is used. In this work, particle surface friction and rotation are considered explicitly. In order to describe the solid phase rheology thoroughly, an extra energy balance equation for the fluctuating rotational kinetic energy of the solids was derived by Yang et al. [24].

$$\begin{aligned}\frac{3}{2}\left[\frac{\partial(\varepsilon_s\rho_s\Theta_t)}{\partial t}+\nabla\cdot(\varepsilon_s\rho_s\mathbf{v}_s\Theta_t)\right]=&-\nabla\mathbf{v}_s\\&:(P_s\mathbf{I}+\varepsilon_s\boldsymbol{\tau}_s)-\varepsilon_s\nabla\cdot(-\kappa_t\nabla\Theta_t)-\gamma_t-3\beta_A\Theta_t\end{aligned} \tag{5}$$

$$\frac{3}{2}\left[\frac{\partial(\varepsilon_s\rho_s\Theta_r)}{\partial t}+\nabla\cdot(\varepsilon_s\rho_s\mathbf{v}_s\Theta_r)\right]=-\varepsilon_s\nabla\cdot(-\kappa_{r1}\nabla\Theta_r-\kappa_{r2}\nabla\Theta_t)-\gamma_r \tag{6}$$

Definitions of the translational granular temperature Θ_t and rotational granular temperature Θ_r are $\Theta_t\equiv\langle C^2\rangle/3$, $\Theta_r\equiv I\langle\Omega^2\rangle/3m$, where I is the particle's moment of inertia. The full expressions for the constitutive equations are summarized in Table 1.

3. Model validation

3.1. Simulation settings

Comparisons between DPM and TFM simulation results will be presented to validate the newly-built kinetic theory. In the simulations, a no-slip wall boundary condition for side walls (left, right, front and back side of the rectangular domain) is used for the gas phase. At the bottom inlet, a uniform gas velocity is specified, whereas at the top outlet, atmospheric pressure (101,325 Pa) is prescribed. For the solid phase, a partial slip boundary condition is used for the side walls. A relation for the solids velocity gradient and an expression for the pseudo Fourier fluctuation energy flux at the wall have been given by Sinclair and Jackson [27]. At high solids volume fraction, we employed the frictional stress model from Srivastava and Sundaresan [30] to account for dense packing. The simulation settings are specified as follows in Table 2.

Table 1
Closure equations of the new kinetic theory of granular flow with friction (model A).

Solid pressure tensor: $P_s=\varepsilon_s\rho_s\Theta_t[1+2(1+e)\varepsilon_s g_0]$
Bulk viscosity: $\lambda_s=\frac{4}{3}\varepsilon_s\rho_s\sigma g_0(1+e)\sqrt{\frac{\Theta_t}{\pi}}$
Solid stress tensor: $\boldsymbol{\tau}_s=-\{(\lambda_s-\frac{2}{3}\mu_{t_s})(\nabla\cdot\mathbf{v}_s)\mathbf{I}+\mu_{t_s}[\nabla\mathbf{v}_s+(\nabla\mathbf{v}_s)^T]+\mu_{r_s}[\nabla\mathbf{v}_s-(\nabla\mathbf{v}_s)^T]\}$
Translational energy dissipation: $\gamma_t=\Theta_t g_0\rho_s\varepsilon_s^2\left\{\begin{array}{l}-\frac{192}{\sigma}\sqrt{\frac{\Theta_t}{\pi}}[\eta_1(1+\eta_1)-(2\lambda+1)A_1\\+(\lambda+1)A_2]+12\nabla\cdot\mathbf{v}_s[\eta_1(1+\eta_1)\\+5[(\lambda+1)A_4-(2\lambda+1)A_3]\end{array}\right\}$ (T1)
Rotational energy dissipation rate: $\gamma_r=\Theta_t g_0\rho_s\varepsilon_s^2\{-\frac{96}{\sigma}\sqrt{\frac{\Theta_t}{\pi}}(2.5A_2-\lambda A_1)+120\nabla\cdot\mathbf{v}_s(2.5A_4-\lambda A_3)\}$ (T2)
Translational shear viscosity: $\mu_{t_s}=\overline{\mu}(1+\mu_{t_{s,c}})+\frac{3}{5}\lambda_s,\mu_{t_{s,c}}=-\frac{4}{5}\varepsilon_s g_0[-6(2\lambda+1)A_1+2\eta_1]$
Rotational shear viscosity: $\mu_{r_s}=-8(2\lambda+1)\sigma g_0\rho_s\varepsilon_s^2 A_1\sqrt{\frac{\Theta_t}{\pi}}$
Translational thermal conductivity: $\kappa_t=\overline{\kappa}_t(1+\kappa_{t_{s,c}})+\frac{3}{2}\lambda_s,\ \ \kappa_{t_{s,c}}=-\varepsilon_s g_0(2\eta_1-16(2\lambda+1)A_1)$
Rotational thermal conductivity: $\kappa_{r1}=\overline{\kappa}_{r,1}=\rho\Theta_t(L_3/2L_1),\kappa_{r2}=\overline{\kappa}_{r,2}=\rho\Theta_t(L_2/2L_1)$,
$L_1=\frac{-32\varepsilon_s g_0}{25\sigma}\sqrt{\frac{\Theta_t}{\pi}}[50A_2/\lambda-10A_1-10A_{11}/3-50(\lambda+1)(\lambda+2)A_{12}/(3\lambda)+10(3\lambda+4)A_9/3]$
$L_2=g_0\varepsilon_s\Theta_t[\frac{56\eta_1\lambda(\lambda+2)}{5(\lambda+1)}-60(1+4\eta_1)(2A_3\lambda-5A_4)]$
$L_3=(1+\frac{12}{5}g_0\varepsilon_s)\lambda\Theta_t[-\frac{8\eta_1(2+\lambda)}{3(1+\lambda)}+50(1+\eta_1)A_3]$

Here, λ is the granular temperature ratio. The expressions for A_1, A_2, A_3, A_4, A_9, A_{11}, and A_{12} can be found in Appendix A. For spheres, $\lambda=2.5\Theta_r/\Theta_t$, $\eta_1=-(1+e)/2$, $\eta_2=-(1+\beta_0)/7$.

3.2. Results and discussion

3.2.1. Influence of normal restitution coefficient

Fig. 1 shows a comparison of time-averaged axial particle velocity and solids volume fraction using different normal restitution coefficients. In all cases a solids circulation pattern emerges, in which small bubbles increase rapidly in size due to coalescence. Consequently, a zone of increased bubble development, initially close to the wall, moves towards the center of bed with increasing height above the gas inlet. Zones with high solids volume fraction near the lateral walls and bottom of the bed are observed in both DPM and TFM model A, while no dense zone near the bed bottom is present in TFM model B. Particles appear to move upwards in regions of more intense bubble activity and downwards in regions of lesser bubble activity, which results in the formation of a pronounced global solids circulation pattern in all models. Both solids circulation pattern and distribution are not very sensitive with respect to the normal restitution coefficient. Comparing with

Table 2
Properties of particle and settings.

Parameters	DPM	TFM
Particle	Glass (ρ = 2526 kg/m^3), σ = 2 mm	Same
Initial bed height	0.15 m	Same
Domain size	0.15 × 0.012 × 0.48 m	Same
Initial bed voidage	0.403	Same
Grid number (x × y × z)	25 × 2 × 80	Same
Normal spring stiffness	k_n = 12.000 N/m	–
Particle-particle collision	e = 0.97, 0.9, β_0 = 0.33, μ = 0, 0.05, 0.15	Same
Particle-wall collision	e_w = 0.97, β_w = 0.33, μ_w = 0.1	–
Specularity coefficient	–	0.1
Simulation time	25 s	Same
Superficial gas velocity	2.27 m/s	Same
Drag relation	Ergun [28], and Wen & Yu [29]	Same
Frictional viscosity model	–	Srivastava and Sundaresan [30]
Flow solver time step	10^{-4} s	Same
Solid phase time step	10^{-5} s	10^{-4} s