International Journal of Multiphase Flow 71 (2015) 1–13

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmulflow

# Influence of collisional parameters for rough particles on simulation of a gas-fluidized bed using a two-fluid model

Yunhua Zhao *, Bing Lu, Yingjie Zhong

*College of Mechanical Engineering, Zhejiang University of Technology, Hangzhou 310014, China*

ARTICLE INFO

*Article history:*
Received 26 January 2014
Received in revised form 6 September 2014
Accepted 19 December 2014
Available online 31 December 2014

*Keywords:*
Friction coefficient
Restitution coefficient
Kinetic theory
Boundary conditions
Bubbling fluidized bed
Two-fluid model
Numerical simulation

ABSTRACT

Three physically realistic collisional parameters, the friction coefficient and the normal and tangential restitution coefficients, are used to characterize the rough particle collisions. The corresponding kinetic theory model and boundary conditions are incorporated into a two-fluid model to investigate the influence of these collisional parameters on the numerical simulation of a gas–solid bubbling fluidized bed. The simulated results reveal that coefficients of friction and normal restitution play important roles in the formation of heterogeneous structures in the bubbling bed, but their inherent effects on particle motion and bed expansion are quite different. In addition, the time-averaged gas–solid flow fields for different friction coefficients vary significantly, but those for different normal restitution coefficients exhibit very similar patterns. To achieve a better agreement with the experimental data, adjusting the friction coefficient is more effective than refining the normal restitution coefficient. The tangential restitution coefficient has relatively weak but non-monotonic effects on particle motion and bed expansion, and the flow fields for different tangential coefficients remain almost the same. Distinct effects of particle–particle and particle–wall collisions are also studied. For the overall fluidization behavior in a small-scale bubbling bed, the most crucial parameter is the friction coefficient for particle–wall collisions, followed by the normal restitution coefficient of particle–particle collision.

## Introduction

In recent years, computational fluid dynamic (CFD) has become an effective tool to study gas–solid fluidization (Tsuji, 2007; Van der Hoef et al., 2008). Among these CFD simulations, the discrete element model (DEM, based on soft-sphere interactions), discrete particle model (DPM, based on hard-sphere collisions) and two-fluid model (TFM, based on pseudo-fluid rheology) are widely used, and the TFM is believed to be a promising tool due to its compromise between computational cost, level of detail provided and potential of applicability (Sundaresan, 2000; Liu et al., 2010; Loha et al., 2013).

In the TFM, the solid phase rheology and the gas–solid interactions require additional constitutive relations and closure laws. Kinetic theory of granular flow is commonly applied to derive the constitutive relations for the dense particulate phase. In the original kinetic theory model (Jenkins and Richman, 1985; Gidaspow, 1994; Enwald et al., 1996), particles are assumed to be perfectly smooth spheres, and particle–particle collisions can be described by a single parameter. Only the normal impact and rebound velocities of two colliding particles are related using the coefficient of normal restitution, while the particle velocity changes in the tangential direction are neglected. The sensitivity and significance of the normal restitution coefficient in modeling gas–solid fluidized beds have been investigated by many researchers (e.g., Goldschmidt et al., 2001; Taghipour et al., 2005; Reuge et al., 2008; Wang et al., 2010b; Chalermsinsuwan et al., 2012).

In realistic systems, the surfaces of particles are rough, thus particle–particle collisions will definitely cause changes to the tangential velocities. Coulomb's law of friction is suitable to describe the frictional interaction of the particles. Abu-Zaid and Ahmadi (1990) used a friction coefficient to describe the collisional slip-friction and developed a kinetic theory model for extremely small particles. It was shown that if frictional interaction was included, the model predictions were in good agreement with experimental and simulation data (Abu-Zaid and Ahmadi, 1993). However, the slip-friction does not reflect the consequences of elasticity associated with tangential deformations of the particles. On the other hand, in many previous efforts to incorporate frictional collisions into a kinetic theory model (e.g., Lun, 1991; Goldshtein and Shapiro, 1995; Songprawat and Gidaspow, 2010; Wang et al., 2012), the roughness coefficient or the so called tangential restitution coefficient was used to characterize the ratio of

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* Corresponding author. Tel./fax: +86 571 88320650.
*E-mail address:* zhaoyh@zjut.edu.cn (Y. Zhao).

http://dx.doi.org/10.1016/j.ijmultiphaseflow.2014.12.002
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tangential relative velocity of the point of contact after a collision to its value before a collision. In fact, the roughness coefficient is a mixed approximate expression for both friction and tangential restitution, and a fixed value for the roughness coefficient can only provide an averaged and simplified description over a spectrum of collisions (Goldshtein and Shapiro, 1995). So far the value of the roughness coefficient still remains difficult to be properly measured from experiments, although its sensitivity and importance have been demonstrated in validation studies of gas–solid fluidization (Wang et al., 2008, 2012; Hao et al., 2010; Songprawat and Gidaspow, 2010).

According to Walton (1993), a more realistic collision operator can be distinguished between sliding and sticking collisions. In a sliding collision, the normal restitution coefficient and the friction coefficient are used to relate the normal and tangential relative velocities before and after a collision; in a sticking collision, the normal restitution coefficient and a constant tangential restitution coefficient are used instead. Since these three coefficients are measurable and could give a reasonably accurate description of experiments performed with real particles (Foerster et al., 1994; Lorenz et al., 1997; Wu et al., 2008), they are widely applied in discrete particle modeling of gas–solid fluidized beds (e.g., Hoomans et al., 1996; Van Wachem et al., 2001; Zhou et al., 2002; Huilin et al., 2005; Mezhericher et al., 2012; He et al., 2012). Based on these physically realistic coefficients, a simple kinetic theory for flow of slightly frictional and nearly elastic particles was derived by Jenkins and Zhang (2002), and then incorporated into TFM to study the gas–solid fluidization by many researchers, such as Goldschmidt et al. (2004), Sun and Battaglia (2006), Shuyan et al. (2008), Benyahia (2008), Liu et al. (2011), Yusuf et al. (2012) and Verma et al. (2013). However, to the present authors' knowledge, no systematic study on the influence and sensitivity of the three collisional coefficients on TFM simulations of gas–solid fluidization has been reported.

In addition, the wall boundary conditions induced by particle–wall collisions are believed to be crucial to the quantitative prediction of gas–solid flows as indicated, for example, by Benyahia et al. (2005), Almuttahar and Taghipour (2008), Artoni et al. (2011), and Lan et al. (2012). In general, there are two main approaches for incorporating the physics of particle–wall collisions into the kinetic theory model. Johnson and Jackson (1987) proposed wall boundary conditions in a heuristic way by using the normal restitution coefficient and a specularity coefficient. Similarly to the roughness coefficient, the specularity coefficient includes the effects of wall roughness and particle–wall friction. This causes great difficulties for measurements, thus no experimental value of the specularity coefficient is reported in the open literature. However, many studies confirmed that the gas–solid flow field is very sensitive to the specularity coefficient (Li et al., 2010; Chalermsinsuwan et al., 2012; Benyahia, 2012; Loha et al., 2013; Li and Benyahia, 2013). In contrast, Jenkins (1992) proposed boundary conditions by employing measurable properties, which are actually the normal and tangential restitution coefficients and the friction coefficient of particle–wall collisions. The boundary conditions by Jenkins (1992) were expressed for two asymptotic circumstances, namely the small-friction limit and the large-friction limit. Jenkins and Louge (1997) improved those expressions and suggested that the appropriate boundary conditions could be obtained by interpolating between those two limits. Based on the theory of Sommerfeld and Huber (1999) and data of Louge (1994), Schneiderbauer et al. (2012) recently extended the boundary conditions for a broad range of collisional properties. Yet the influences of the three particle–wall collisional coefficients on the gas–solid fluidization have not received enough research attention. It is worth mentioning that structural wall roughness can be also involved in modeling particle–wall collisions within the Euler–Lagrange framework (Sommerfeld, 2003; Sommerfeld and Kussin, 2003; Laín and Sommerfeld, 2008; Breuer et al., 2012). In gas–solid fluidization, the scales of wall roughness are commonly negligible compared to the sizes of particles, thus the structural wall roughness and a resulting so-called shadow effect (Sommerfeld and Huber, 1999) are beyond the scope of this paper.

In this paper, both the particle–particle and particle–wall collisions are characterized by the friction coefficient and the normal and tangential restitution coefficients, the corresponding constitutive relations (Section Kinetic theory of rough particles) and wall boundary conditions (Section Wall boundary conditions for the solid phase) are based on the kinetic theory of rough particles proposed by the authors (Zhao et al., 2013). The objective of this study is to investigate the sensitivities of these collisional parameters through two-fluid modeling of a gas–solid bubbling fluidized bed. With this in mind, simulations with different collisional parameters are carried out and analyzed. The computed particle velocity and volume fraction distributions are also compared with the magnetic resonance (MR) measurements by Müller et al. (2008, 2009).

## Model description

### *Basic two-fluid model*

In the TFM, the solid phase is described as a continuum, just like the gas phase. The continuity equations for gas and solid phases are given by

$$\frac{\partial}{\partial t}(\varepsilon_i\rho_i) + \nabla\cdot(\varepsilon_i\rho_i\mathbf{u}_i) = 0 \tag{1}$$

where $t$ is time, $\varepsilon$, $\rho$ and $\mathbf{u}$ represent the local volume fraction, density and velocity vector, respectively. The subscript $i = g$ for the gas phase and $i = s$ for the solid phase.The momentum conservation equations are given by

$$\frac{\partial}{\partial t}(\varepsilon_g\rho_g\mathbf{u}_g) + \nabla\cdot(\varepsilon_g\rho_g\mathbf{u}_g\mathbf{u}_g) = \nabla\cdot(\varepsilon_g\boldsymbol{\tau}_g) - \varepsilon_g\nabla p_g - K(\mathbf{u}_g - \mathbf{u}_s) + \varepsilon_g\rho_g\mathbf{g} \tag{2}$$

$$\frac{\partial}{\partial t}(\varepsilon_s\rho_s\mathbf{u}_s) + \nabla\cdot(\varepsilon_s\rho_s\mathbf{u}_s\mathbf{u}_s) = \nabla\cdot\boldsymbol{\tau}_s + \nabla p_s - \varepsilon_s\nabla p_g + K(\mathbf{u}_g - \mathbf{u}_s) + \varepsilon_s\rho_s\mathbf{g} \tag{3}$$

where $p$ is the hydrodynamic pressure, $\mathbf{g}$ is the gravity vector, $\boldsymbol{\tau}$ is the shear stress tensor and $K$ is the momentum exchange coefficient caused by the drag force between gas and solid phases.

The stress tensor for the gas or solid phase can be written in a general form as

$$\boldsymbol{\tau}_i = \mu_i(\nabla\mathbf{u}_i + \nabla\mathbf{u}_i^T) + \left(\xi_i - \frac{2}{3}\mu_i\right)(\nabla\cdot\mathbf{u}_s)\mathbf{I} \tag{4}$$

where $\mu$ and $\xi$ are the shear and bulk viscosity, and $\mathbf{I}$ is the identity tensor. The bulk viscosity quantifies the resistance of a fluid to rapid compression, and is often set to zero for a low-speed gas flow. The viscosity and the pressure of the solid phase can be specified via kinetic theory of granular flow or empirical formulae (Enwald et al., 1996). In this work, the kinetic theory approach is used to describe the solid phase properties on a more fundamental basis (see the next subsection).

There are many different models for the momentum exchange coefficient in the literature. To simulate the dense gas–solid flow in fluidized beds, the Gidaspow (1994) model is applied as follows: