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Euler–Euler modeling of a gas–solid bubbling fluidized bed with kinetic theory of rough particles

Yunhua Zhao*, Bing Lu, Yingjie Zhong

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

HIGHLIGHTS

- Kinetic theory of rough particles is developed.
- Three parameters are adopted to characterize the rough particle collisions.
- Both the translational and rotational granular temperature equations are solved.
- Flat wall boundary conditions for rough particles are proposed.
- Bubbling fluidized beds with rough and smooth particles are simulated and compared.

ARTICLE INFO

ABSTRACT

Kinetic theory of granular flow is extended for rough particles. Both the translational and rotational granular temperatures are introduced to characterize the random fluctuations of particles. Sliding and sticking mechanisms are distinguished in the binary collision model with the friction coefficient and coefficients of normal and tangential restitution. Collision integrals are performed to produce new expressions of the constitutive relations for rough particles. Flat wall boundary conditions for rough particles are proposed according to the particle–wall collisions. The present model is incorporated in Euler–Euler simulations of a bubbling gas–solid fluidized bed. The computed bed expansion dynamics and flow patterns are validated with experimental measurements and Euler–Lagrange simulations. The ratio of rotational to translational granular temperatures is found to be influenced by the particle volume fraction and the fluidization velocity. Comparison among the present model, the original smooth particle model and another rough particle model is also carried out.

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1. Introduction

Gas–solid fluidized beds are widely used in combustion, gasification, catalytic cracking and metallurgical processes. The success of such systems relies primarily on their fluid dynamic behavior. So a sound understanding of the mechanisms governing the complex flow phenomena involved in fluidized beds is a key issue in improving system efficiency and reliability.

In the past several decades, computational fluid dynamics (CFD) has emerged as an effective tool for fundamental research and industrial design of fluidized bed applications. Two approaches are frequently used for CFD modeling of gas–solid fluidized beds; namely, the Euler–Lagrange (EL) approach and the Euler–Euler (EE) approach. In the Euler–Lagrange approach (Tsuji et al., 1993; Hoomans et al., 1996), the gas phase is treated as a continuous phase and is described by locally averaged Navier–Stokes equations on a computational cell scale; whereas the solid phase is treated as discrete particles, and described by Newton's laws of motion on a single particle scale. A comprehensive review of the EL approach as well as their application in gas–solid flows can be found in the literature (for example, Deen et al., 2007; Zhu et al., 2007). The strength of the EL approach is that it allows studying the individual particle motion and particle–particle interactions directly, but the main obstacle is the huge demand of computing resources, which at the present constrains its application in large systems of particles. In the EE approach (Gidaspow, 1994; Enwald et al., 1996; Kuipers and van Swaaij, 1998), both the gas and solid phases are assumed as fully inter-penetrating continua, and are described by separate conservation equations for mass and momentum. Owing to the continuum representation of the particulate suspension, the EE approach is not limited by the particle number, and becomes a more natural choice for hydrodynamic modeling of engineering scale systems (van Wachem et al., 2001; van de Hoef et al., 2004). However, additional closure equations are required in the Euler–Euler approach to describe the rheology of the solid phase.

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

Within the framework of the EE approach, kinetic theory of granular flow (KTGF) is commonly used to obtain constitutive relations for the solid phase. This theory is basically an extension of the classical kinetic theory of non-uniform gases (Chapman and Cowling, 1970) to dense particulate flows. One important difference between solid particles and gas molecules is that kinetic energies are conserved in molecule collisions, but dissipated in particle collisions due to their inelasticity and friction. The original kinetic theory of granular flows (Jenkins and Savage, 1983; Lun et al., 1984; Jenkins and Richman, 1985) assumed solid particles to be smooth spheres, these assumptions led to a decoupling of rotational and translational degrees of freedom, and the resulting theory involved particle translational motion only. In realistic situations, particle surfaces cannot be perfectly smooth. During rough particle collisions, surface friction causes rotational velocity fluctuations. As a result, kinetic energies interchange between translational and rotational modes; furthermore, additional energy can be dissipated through friction.

In many cases, the dynamic effects of particle surface friction and rotary inertia play significant roles and should not be ignored. Lun and Jenkins (1987) started to consider rough spherical particles to study the influence of surface friction of particles. In their article, the frictional property of the surface was characterized by a constant roughness coefficient β, which could range from -1 to 1. When $\beta = -1$, the particle surfaces are perfectly smooth. As β becomes larger, the surfaces become rougher. When $\beta = 1$, the particles are said to be perfectly rough. They derived a simple kinetic theory for granular flow in the dense limit. Two granular temperatures were involved in their kinetic theory, one was translational temperature, which measured the kinetic energy of fluctuations in the translational velocity, and the other one was rotational temperature, which measured the kinetic energy of the fluctuations in rotational velocity. Later Lun (1991) considered the kinetic as well as the collisional contributions for stresses and energy fluxes, and extended the kinetic theory to be appropriate for both dilute and dense granular flows. For simple shear flows, an explicit expression for the ratio of the rotational temperature to the translational temperature was proposed. This explicit expression together with the kinetic theory were adopted by Shuyan et al. (2008b) to compute bubbling fluidized beds and by Zhenhua et al. (2010) to compute circulating fluidized bed risers. In the literature, the roughness coefficient is sometimes named rotational restitution coefficient by Walton (1993) or tangential restitution coefficient by Luding et al. (1998), Kumaran (2006), and Santos et al. (2010, 2011). Most recently, with a constant tangential restitution coefficient, Songprawat and Gidaspow (2010) and Shuai et al. (2011, 2012) followed Goldshtein and Shapiro's (1995) way of combining the translational and rotational granular temperatures into a total granular temperature, and developed a kinetic theory of rough particles for computation of gas–solid flows. Besides the roughness coefficient, the practical particles always have a constant Coulomb friction coefficient, μ. Abu-Zaid and Ahmadi (1990) introduced the friction coefficient into the kinetic model to account for frictional losses during particle–particle collisions. They assumed that particles were sufficiently small such that the particle-spin effects could be neglected. Thus the original kinetic model for smooth particles was modified to include the friction without bringing in additional equation of conservation. Their model was used to analyze several rapid flow problems and showed better agreement with the experimental data (Abu-Zaid and Ahmadi, 1993).

In fact, the value of β depends on particle inelasticity, surface friction and geometry of the collision. When sliding (slip) contact occurs, Coulomb's law of friction is suitable to describe the interaction. Therefore, Walton (1993) and Lun and Bent (1994) distinguished between sliding and sticking (no-slip) collisions, for a sliding collision, they used Coulomb friction coefficient μ to describe the friction mechanics; while for a sticking collision, a phenomenological constant β_0 was used. Since this method could give a reasonably accurate description of experiments performed with real particles (Maw et al., 1981; Foerster et al., 1994; Lorenz et al., 1997), it is nowadays widely applied in Euler–Lagrange simulations with the hard-sphere model. Jenkins and Zhang (2002) derived a simple kinetic theory for rough spherical particles based on these physically realistic parameters. When the friction coefficient was small, they solved the conservation equations for rotational momentum and temperature approximately, hence, the resulting theory had the same structure as that for smooth particles, the only modification was the introduction of additional dissipation terms in the translational temperature equation and its boundary condition. This simple way to incorporate particle friction and rotation into the kinetic theory was implemented by Goldschmidt et al. (2004), Jin and Francine (2006) and Shuyan et al. (2008a) to study the fluid dynamic behaviors in dense fluidized beds.

In this study, the kinetic theory of granular flow is extended for rough particles to include the state-of-the-art particle collision mechanism and particle rotational dynamics. The kinetic theory model is incorporated in Euler–Euler simulations of a bubbling gas–solid fluidized bed. The computed results are validated with Euler–Lagrange simulations and experimental measurements by Goldschmidt et al. (2004). Comparison among the present model, the original kinetic theory model and the Jenkins and Zhang (2002) model is also carried out.

2. Model description

2.1. Laws of conservation

Given a particle property ϕ, which is a function of particle translational velocity $\mathbf{c}$ and rotational velocity $\boldsymbol{\omega}$, its averaged value at position $\mathbf{x}$ and time t is calculated using the single particle velocity distribution function $f(\mathbf{c}, \boldsymbol{\omega}, \mathbf{x}, t)$:

$$\langle \phi \rangle = \frac{1}{n} \int \phi f(\mathbf{c}, \boldsymbol{\omega}, \mathbf{x}, t) d\mathbf{c} d\boldsymbol{\omega} \tag{1}$$

where n is the local number density of particles and can be obtained by setting $\phi = 1$ in the above equation.

Then, at $\mathbf{x}$ and t, the mean translational velocity $\mathbf{u} = \langle \mathbf{c} \rangle$ and the mean rotational velocity $\boldsymbol{\varpi} = \langle \boldsymbol{\omega} \rangle$. The fluctuations for translational and rotational velocities are given by $\mathbf{C} = \mathbf{c} - \mathbf{u}$ and $\boldsymbol{\Omega} = \boldsymbol{\omega} - \boldsymbol{\varpi}$, respectively. Thereby, the translational granular temperature is defined by $T = \langle C^2 \rangle / 3$, and the rotational granular temperature by $\Theta = I \langle \Omega^2 \rangle / 3m$, where m denotes the particle mass and I denotes the moment of rotary inertia.

Considering a population of identical particles, a conservation equation for the number of particles in a volume element can be formulated in terms of a single particle velocity distribution function to yield the Boltzmann equation (Chapman and Cowling, 1970). Multiplying the particle property ϕ with the Boltzmann equation and integrating over all range of velocities $\mathbf{c}$ and $\boldsymbol{\omega}$, one obtains the conservation equation for $\langle \phi \rangle$, as proposed by Jenkins and Zhang (2002) and Yoon and Jenkins (2005):

$$\frac{Dn\langle\phi\rangle}{Dt} + n\langle\phi\rangle\frac{\partial u_i}{\partial x_i} + \frac{\partial n\langle C_i\phi\rangle}{\partial x_i} + n\frac{D\langle c_i\rangle}{Dt}\left\langle\frac{\partial\phi}{\partial C_i}\right\rangle - n\left\langle F_i\frac{\partial\phi}{\partial C_i}\right\rangle$$
$$+ n\left\langle\frac{\partial\phi}{\partial C_i}C_j\right\rangle\frac{\partial u_i}{\partial x_j} + n\frac{D\varpi_i}{Dt}\left\langle\frac{\partial\phi}{\partial\Omega_i}\right\rangle + n\left\langle\frac{\partial\phi}{\partial\Omega_i}C_j\right\rangle\frac{\partial\varpi_i}{\partial x_j} = \chi(\phi)$$
$$- \frac{\partial\psi_i(\phi)}{\partial x_i} - \frac{\partial u_i}{\partial x_j}\psi_j\left(\frac{\partial\phi}{\partial C_i}\right) - \frac{\partial\varpi_i}{\partial x_j}\psi_j\left(\frac{\partial\phi}{\partial\Omega_i}\right) \tag{2}$$

where F is the external body force per unit of mass acting on particles, and the right-hand side terms describe the collisional