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CFD simulation of bubbling fluidized beds using kinetic theory of rough sphere

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ABSTRACT

Flow behavior of particles is simulated using an Eulerian–Eulerian two-fluid model based on the kinetic theory of rough spheres. The interactions of the short and fast collisions of particles are incorporated to consider the redistribution of momentum and kinetic energy between the collision and friction interactions. The fluctuating kinetic energy by collisions of particles has taken the transfer of particle kinetic energy between the rotational and translational degrees of freedom and also the energy losses into account. Two coefficients, normal restitution coefficient and tangential restitution coefficient, are used to characterize the collisions of particles. The friction coefficient is used to predict the frictional stresses caused by the enduring contacts of particles. The collisional and frictional constitutive relations are used to predict the stresses of rough spheres. The solid pressure and viscosity are obtained in terms of the normal and tangential restitution coefficients and empirical friction constants. Distributions of concentrations and velocities of particles are predicted in the 2-D bubbling fluidized bed. The influence of bed temperature and particle diameter on fluctuation kinetic energy is analyzed in the bubbling fluidized beds. Simulated results are compared with measured axial velocity of particles and bubble diameter published in literature.

1. Introduction

The kinetic theory of granular flow (KTGF) was widely used to simulate flow behavior of particles in the bubbling fluidized beds. This theory is basically an extension of the classical kinetic theory of dense gases (Chapman and Cowling, 1970) to particulate flows, that takes non-ideal particle–particle collisions and gas–particle drag into account. Gidaspow (1994) generalized the kinetic theory of granular flow to gas–particle flows. An important difference is that collisions between molecules in the dense gas are considered as elastic whereas the particle collisions are inelastic causing kinetic energy dissipating into heat. Associated with the random motion of the particles, a granular temperature θ is defined as $\theta = \langle \mathbf{CC} \rangle /3$ where $\mathbf{C}$ is the random fluctuating translational velocity of particles (where $\langle\ \rangle$ denotes ensemble averaging). Modeling of the collisional and kinetic transport mechanisms for the momentum and fluctuating kinetic energy of particles yield a description of the momentum transport properties as a function of the granular temperature, and an additional transport equation for the kinetic energy of the random motion of the particles describing the granular temperature distribution. However, the original KTGF models of Savage and Jeffrey (1981), Lun et al. (1984) and Jenkins and Richman (1985) as well as the generalized model of Gidaspow (1994) are derived for smooth, rigid, nearly elastic, spherical particles ($1.0-e$ must be small, where e is the coefficient of normal restitution) in translational motion, and do not allow for particle rotation. In realistic situation, particle surface cannot be perfectly smooth and particles are frictional as well as inelastic. In many practical systems, the rough, inelastic particles are encountered, which makes application of the original KTGF models questionable. Therefore, the effect of friction on motion of particles must be considered in the numerical simulations.

During a collision of rough particles, the fluctuation energy is dissipated from inelasticity and frictions. The frictional particle collision also results in the particle rotation, which gives additional loss of the energy. As a result, particles can rotate with angular velocity $\boldsymbol{\omega}$ under rapid rates of deformation. Jenkins and Mancini (1987) studied kinetic theory for rough, inelastic spherical particles. In the kinetic theory for flow of identical, slightly frictional, inelastic spheres proposed by Lun (1991) and Jenkins and Zhang (2002), two granular temperatures are involved. The first is the translational granular temperature θ_t, which measures the energy associated with the translational velocity fluctuations, defined as $\theta_t = \langle \mathbf{C}^2 \rangle /3$. The second is the rotational granular temperature θ_r, which measures the energy associated with the

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angular velocity fluctuations, defined as $\theta_r = (1/3m)I_p\langle(\mathbf{\Omega})^2\rangle$, where I_p is the moment of inertia, $\mathbf{\Omega}$ is the angular velocity fluctuation and m is the mass of a particle. The conservation equations of the mass, linear momentum, mean particle spin, particle translational and rotational fluctuation kinetic energies are involved. The kinetic energies associated with fluctuations in both translational velocity and spin are considered. The additional equations for angular momentum and rotational granular energy greatly increase the complexity of the kinetic theory, and are often difficult to apply to general flows. Collisional motion of rough inelastic spheres was analyzed on the basis of the kinetic Boltzmann–Enskog equation (Goldshtein and Shapiro, 1995). The Chapman–Enskog method for gas kinetic theory is modified to derive the Euler-like hydrodynamic equations for a system of moving spheres, possessing constant roughness and inelasticity. Sun and Battaglia (2006) implemented a model from kinetic theory for rapid flow of identical, slightly frictional, nearly elastic spheres (Jenkins and Zhang, 2002) into the MFIX CFD code (Syamlal et al., 1994). In this model, 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 momentum and translational energy is negligible. Only the dissipation rates for translational and rotational granular energy are influenced by friction. They found that the model captures the bubble dynamics and time-averaged bed behavior. Shuyan et al. (2008) simulated flow behavior of particles in the bubbling fluidized bed based on the kinetic theory for flow of dense, slightly inelastic, slightly rough sphere proposed by Lun (1991) to account for rough sphere binary collisions. Zhenhua et al. (2010) studied the effect of roughness coefficient on flow behavior of particles in risers. Simulated results show that the simulated energy dissipation, granular temperature, viscosity and thermal conductivity of particles exhibit nonmonotonic roughness coefficient dependencies due to the energy conversion resulting from the collisions and rotation of particles.

In the bubbling fluidized beds, the local concentration of particles may be high, and particles become closer. The period of interaction is no longer instantaneous. The kinetic and the plastic stresses caused by interaction of particles are equally important. Particles exhibit behavior similar to that of a rigid solid. When applying a stress to a bulk assembly of particles the strain or deformation rate is induced. This bulk assembly of particles can display elastic and plastic behavior as the stress on the particles increases. By adopting theories mainly arising from the study of soil mechanics (e.g., Schaeffer, 1987; Tardos, 1997), several theories for describing the stresses in the plastic flow regime have been proposed. Johnson and Jackson (1987) proposed to sum the stresses obtained from the kinetic theory to the frictional stresses provided by the frictional stress model, being able to capture the two extrema of the behavior of the flow (viscous flow and plastic flow). Srivastava and Sundaresan (2003) adopted the additive approach of Johnson and Jackson (1987) with an expression for the asymmetric part of the stresses derived from Schaeffer (1987), modified to account for strain rate fluctuations in the quasi-static flow. This kinetic-frictional stresses model provides a relationship to determine the solid stresses as a function of the solid strain rates. Numerical simulations showed that the frictional stress considerably influences on the concentration of particles in the spouted bed (Huilin et al., 2004) and the shape of the bubble in the bubbling fluidized beds (Patil et al., 2005; Makkawi and Ocone, 2006; Passalacqua and Marmo, 2009; Vun et al., 2010). This is important for the Eulerian–Eulerian method as the momentum equation for the solid phase requires closure terms for the solid stresses.

The KTGF models mentioned above have developed and implemented the quasi-static model for the solid stresses in dense regions into fluidized bed models. On the other hand, there is a relatively limited number of studies dealing with the energy dissipation due to the rotation of particles. The present work, therefore, aims to incorporate the frictional stresses model and the additional energy dissipation due to frictional collisions into the hydrodynamic model in bubbling fluidized beds. The particle average fluctuation kinetic energy is introduced to govern the mechanism dominating kinetic energy transformation in flow of particles. The conservation equation of fluctuating kinetic energy is proposed to take the transfer of particle fluctuating kinetic energy between the rotational and translational degrees of freedom into account. The kinetic-frictional stress model is used to predict the solid pressure and viscosity of particles. Distributions of concentrations and velocities of gas and particles are predicted in the bubbling fluidized bed. Computed results are compared with axial velocity of particles measured by Laverman et al. (2008). The effect of bed temperature and particles diameter on fluctuation kinetic energy is analyzed.

2. Kinetic theory for granular flow of rough sphere (KTRS)

2.1. Governing equations

In an Eulerian–Eulerian two-phase model, the gas and solids phases are treated as interpenetrating continua, identified by their phase fraction, and exchanging properties like momentum and energy. Each of these continua is described by means of the continuity and momentum equations. The governing equations for the gas phase can be derived by using a suitable volume averaging procedure, while the particle phase transport equations originate from the Maxwellian average of a single-particle quantity over the Boltzmann integral–differential equation (Gidaspow, 1994).

Table 1 shows a summary of the basic equations (Shuai et al., 2011). The continuity equation of gas phase is shown in Eq. (T1-1) without reactions. The gas phase momentum equation is shown in Eq. (T1-3) including an interphase momentum transfer term, where the gas–phase stress tensor τ_g is calculated according to Newton's expression of Eq. (T1-6) (Gidaspow, 1994). β_{gs} is the interphase momentum exchange coefficient.

The continuity equation of solids phase is shown in Eq. (T1-2). The particle phase momentum equation is similar to the one for the gas phase, but contains the gradient of the particle pressure, in addition to the gas pressure gradient multiplied by the concentration of particles. The momentum conservation equation for solids phase is given by Eq. (T1-4), where τ_s the stress tensor of particles.

In a collision between frictional spheres, the collisional impulse has a tangential component and a normal component. The change in the normal velocity is determined by the normal restitution coefficient e, which can range from 0.0 to 1.0. The change in the spin and in the tangential velocity depends on the frictional properties of the surfaces. The frictional properties of the surface are characterized by the tangential restitution coefficient β (Lun and Savage, 1987; Jenkins and Zhang, 2002). A coefficient of tangential restitution, $-1.0 \le \beta \le 1.0$, was used to characterize the ratio of the tangential component of the relative velocity of the point of contact after a collision to its value before a collision.

The fluctuation, $\mathbf{C}$, in translational velocity and the fluctuation, $\mathbf{\Omega}$, in angular velocity are defined by $\mathbf{C} = \mathbf{c} - \mathbf{u}$ and $\mathbf{\Omega} = \boldsymbol{\omega} - \boldsymbol{\varpi}$, respectively, where $\mathbf{u}$ and $\boldsymbol{\varpi}$ are the mean translational velocity and the mean angular velocity, respectively. $\mathbf{c}$ and $\boldsymbol{\omega}$ are the instantaneous translational velocity and the angular velocity of particles, respectively. The mean translational fluctuation kinetic energy is $3m\theta_t/2 = m\langle\mathbf{C}^2\rangle/2$, and the mean rotational fluctuation