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Computational fluid dynamics of riser using kinetic theory of rough spheres

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ABSTRACT

Flow behavior of particles in the riser was simulated using a computational fluid dynamics (CFD). Conservation equations of mass and momentum for solid phase were solved on the basis of kinetic theory of rough spheres (KTRS). The fluctuation kinetic energy of particles is introduced to characterize the random motion of particles as a measure of the translational and rotational velocity fluctuations. The distribution of concentration and velocity of particles are obtained in a riser. The simulated concentration of particles agreed reasonably with the available experimental results. The random-motion kinetic energy of inelastic rough particles is shown to be affected by the particle restitution coefficient and roughness. The effects of the coefficient of normal restitution and roughness on the distribution of solid phase in the riser are studied. In this case, the influence of the coefficient of normal restitution is weak in the riser using KTRS model.

1. Introduction

Flow behavior of gas and particles in fluidized beds is predicted by means of computational fluid dynamics (CFD) tools since CFD models provide a more detailed data profile as a function of space and time. Among different CFD models, the Eulerian–Eulerian (two-fluid) model with kinetic theory of granular flow (KTGF) is the most applicable approach to compute gas–solid flow in circulating fluidized beds [1,2]. In the two-fluid model, the particles are treated as a continuum as in the gas phase. Thus, there are two interpenetrating gas and solid phases where each phase is characterized by its own conservation equation of motion. The interactions between the two phases are expressed as additional source terms added to the conservation equations. The kinetic and collisional momentum transfer due to the collisions of particles is modeled on the basis of the kinetic theory of granular flow (KTGF). This treatment of the particulate phase uses classical results from the kinetic theory of dense gases [3]. This theory gives closures for the rheologic properties of the fluidized particles as a function of the local particle concentration and the fluctuating motion of the particles owing to particle–particle collisions. As kinetic energy of the particles is lost in collisions between pairs of particles, their inelasticity is taken into account through the coefficient of normal restitution. Modeling of the collisional and kinetic transport mechanisms for the momentum and fluctuating kinetic energy of the particles yields a description of the momentum transport properties as a function of the granular temperature. Detailed discussion on the development of KTGF is provided by Gidaspow [1].

In the original KTGF, only smooth spheres in translational motion are considered, and therefore collisions are described with a single constant coefficient of normal restitution, e. In reality, particles are rough and are rotating. This implies that an accurate model considering the effect of friction on motion of particles is required. 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 ω under rapid rates of deformation. The model accounting for friction during collisions assumes, apart from a constant coefficient of normal restitution e, a constant coefficient of tangential restitution β [4]. While e is a positive quantity smaller than or equal to 1 (the value $e=1$ corresponding to elastic spheres), the parameter β lies in the range between -1 (perfectly smooth spheres) and 1 (perfectly rough spheres). The total kinetic energy is not conserved in a collision, unless $e=1$ and $\beta=\pm 1.0$. This implies that an accurate model should be based on at least two coefficients, normal and tangential restitution coefficients in order to be valid for the collision of particles. In the kinetic theory for flow of identical, slightly frictional, inelastic spheres proposed by Lun [5] and Jenkins and Zhang [6], two granular temperatures of particles are involved. The first is translational granular temperature θ_t, which measures the energy associated with the translational velocity fluctuations, defined as $\theta_t = \langle C^2 \rangle/3$, where C is the translational velocity fluctuation of particles. The second is rotational granular temperature θ_r, which measures the energy associated with the angular velocity fluctuations, defined as $\theta_r = (1/3m) I_r \langle \Omega^2 \rangle$, where I_r is the moment of inertia, Ω is the angular velocity fluctuation and m is the mass of a particle. The conservation equations include the mass, linear momentum, spin, translational and rotational fluctuation kinetic energies of particles. The kinetic energies associated with fluctuations in both translational velocity and spin were considered. Thus, 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 proposed by Goldshtein and Shapiro

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[7]. The Chapman–Enskog method is modified to derive the Euler-like hydrodynamic equations for a system of moving spheres, possessing constant roughness and inelasticity. The rough sphere model shows that in contrast to conservative systems, energy is not equipartitioned between the degrees of freedom in dissipative systems, even though the ratio of translational and rotational energy approaches a constant in a freely cooling system [8]. Herbst et al. [9] predicted the rotational and the translational energy dissipation rates for spheres. They employed solutions for the angular momentum balance and the rotational energy balance for a steady homogeneous shearing and incorporated the influence of small friction on the exchange and dissipation of translational fluctuation energy. Yoon and Jenkins [10] indicated the changes in translational and rotational energies associated with either a sticking or a sliding collision. The balance equations for mass, linear and angular momentums, and translational and rotational energies based on the Boltzmann equation were given. The ratio of rotational to translational temperatures is evaluated as the rotational dissipation term is approximated to be zero by ignoring terms involving unsteady and inhomogeneous contributions, as if the flow is in a steady, homogeneous shearing state. Sun and Battaglia [11] implemented a model from kinetic theory for rapid flow of identical, slightly frictional, nearly elastic spheres proposed by Jenkins and Zhang [6] into the MFIX CFD code [12]. 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. [13] 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 [5]. The simulated energy dissipation, granular temperature, viscosity, and thermal conductivity of particles exhibit non-monotonic tangential restitution coefficient dependencies due to the energy losses resulting from particle collisions [14]. Santos et al. [15] evaluate the collisional rates of change of the translational and rotational granular temperature by means of a Sonine approximation. They found that the Maxwellian approximation for the granular temperature ratio does not deviate much from the Sonine prediction in both the homogeneous cooling state and the homogeneous steady state. Recently, the multiphase kinetic theory has been proposed to consider the rotation of particles with unequal masses and diameters [16]. Computations show that the rotation can alter the profiles of velocity and concentration in a riser.

Recently, we proposed a kinetic theory model for rough spheres in the bubbling fluidized beds [17]. In the model for kinetic theory of rough spheres (KTRS), the particle average fluctuation kinetic energy is introduced to govern the mechanism dominating kinetic energy transformation in flow of particles. KTRS takes into account transfer of particle kinetic energy between their rotational and translational degrees of freedom, and also the total energy losses. The model of KTRS has the same structure as that for frictionless spheres, i.e., only conservation of mass, mean translational velocity and particle average fluctuation kinetic energy need to be considered. In present work, KTRS is used to predict flow behavior of particles in a riser. Distributions of concentrations and velocities of gas and particles are predicted. Computed results are compared with experiments measured by Knowlton et al. [18] and Herbert and Reh [19] in risers.

2. Kinetic theory for granular flow of rough sphere

2.1. Governing equations

Considering an ensemble of identical rough spherical particles with spherically symmetric mass distribution, the chaotic translational and rotational motions are assumed in an effectively infinite spatial domain. The fluctuation, **C**, in translational velocity and the fluctuation, Ω, in angular velocity are defined as $\mathbf{C}=\mathbf{c}-\mathbf{u}$ and $\Omega=\omega-\varpi$, respectively, where **u** and ϖ are the mean translational velocity and the mean angular velocity. c and ω are the instantaneous translational velocity and the angular velocity of particles. The inertial properties of each particle are characterized by the moment of rotary inertia I_r, or dimensionless moment of inertia $K=4I_r/(m\sigma^2)$. In particular, for uniform spheres $I_r=0.1m\sigma^2$ and $K=0.4$. The mean translational fluctuation kinetic energy is $3m\theta_t/2=m<C^2>/2$, and the mean rotational fluctuation kinetic energy is $3m\theta_r/2=I_r<\Omega^2>/2$, where θ_t and θ_r are the translational granular temperature and rotational granular temperature. The kinetic energy of random motion of particles, E, is the sum of the translational kinetic energy and the rotational kinetic energy. Thus, the particle fluctuation kinetic energy is

$$e_o=\frac{E}{m}=<\frac{1}{3}C^2+\frac{I_r\Omega^2}{3m}>=(\theta_t+\theta_r) \tag{1}$$

which shows that the kinetic energy involves two measures of the strength of these fluctuations: the translational temperature, and the rotational temperature. In contrast to the definition of fluctuation kinetic energy by Goldshtein and Shapiro [7], the kinetic energy in Eq. (1) includes the translational and rotational contributions. Note that the total granular temperature includes the translational granular temperature and rotational granular temperature. The particle fluctuation kinetic energy e_0 has the units of m^2/s^2. The definition used here is more convenient, since the granular temperature is simply the variance of the measured particle velocity distributions.

For a flow of solid phase, the conservation equations are derived on the basis of the kinetic theory of granular flow. This treatment of the particulate phase uses classical results from the kinetic theory of dense gases [3]. Details are found in Gidaspow [1]. Table 1 lists the equations for flow of gas and solid phases used in present simulations [17].

In an Eulerian–Eulerian two-phase model, the governing equations for the gas phase can be derived by using a suitable volume averaging procedure. The continuity equations of gas phase and solid phase are shown in Eqs. (T1-1) and (T1-2) without reactions. The gas phase momentum equation has the form shown in Eq. (T1-3) as the body force equals to the gravitational acceleration, where the gas-phase stress tensor τ_g is calculated according to Newton's expression of Eq. (T1-6) [1]. The last term on the left-hand side of Eq. (T1-3) represents the interfacial momentum transfer. The momentum conservation equation for solid phase is given by Eq. (T1-4), where τ_s is the stress tensor of particles. The momentum exchange between gas phase and solid phase is represented by the term $\beta_{gs}(\mathbf{u}_g-\mathbf{u}_s)$, where β_{gs} is the drag force coefficient. These equations are the same as that used in the original kinetic theory of granular flow (KTGF) [1]. The correlations for β_{gs} is a combination of Eq. (T1-21) at the gas volume fraction less than 0.8 and Eq. (T1-22) at the gas volume fraction greater than 0.8.

The conservation equation of solid fluctuation kinetic energy e_o is expressed by [17]

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s\rho_s e_o)+\nabla\cdot(\varepsilon_s\rho_s e_o u_s)\right]=\nabla\cdot(\kappa_s\nabla e_o)+(\nabla p_s I+\tau_s) : \nabla u_s-\gamma_s-D_{gs}-3\beta_{gs}e_o. \tag{2}$$

The two terms on the left-hand side of Eq. (2) represent the accumulation and convection of kinetic fluctuation energy, respectively. In the right-hand side of Eq. (2), the first term models the conductive transport of kinetic fluctuation energy. The second term describes the production of kinetic fluctuation energy due to irreversible deformation of the solid phase velocity field. The third term represents the dissipation of the fluctuation energy due to inelastic particle–particle interactions. The fourth term represents the exchange of the fluctuation energy due to interphase momentum transport, and the last term representing the dissipation due to interaction with the fluid.