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Prediction of particle motion in a two-dimensional bubbling fluidized bed using discrete hard-sphere model

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Abstract

The solids motion in a gas–solid fluidized bed was investigated using a discrete hard-sphere model. Detailed collision between particles and a nearest list method are presented. The turbulent viscosity of gas phase was predicted by subgrid scale (SGS) model. The interaction between gas and particles phases was governed by Newton's third law. The distributions of concentration, velocity and granular temperature of particles are obtained. The radial distribution function is calculated from the simulated spatio-temporal particle distribution. The normal and shear stresses of particles are predicted from the simulated instantaneous particle velocity. The pressure and viscosity of particles are obtained from both the kinetic theory of granular flow and the calculated stresses of particles. For elastic particles the individual lateral and vertical particle velocity distribution functions are isotropic and Maxwellian. The observed anisotropy becomes more pronounced with increasing degree of inelasticity of the particles.

Keywords: Discrete hard-sphere approach; Kinetic theory of granular flow; Reynolds stress

1. Introduction

The hydrodynamics of bubbling fluidized bed technology has widespread applications in the petroleum, chemical, and energy industries. Understanding of the fundamental phenomena including the interaction between the particles is needed to improve the design and performance of fluidized beds. Broadly speaking the simulation approaches of two-phase flow in bubbling fluidized bed can be classified into Euler–Lagrange discrete particle trajectory model and Euler–Euler two-fluids model. Several attempts have been made to simulate bubble and particle motion in fluidization using the Eulerian–Lagrangian approach. In this method, the fluid phase is treated as a continuum, while the particles are traced individually by solving the Newtonian equation of motion. The mechanism of particle-to-particle collisions can be described by soft- or hard-sphere models (Crowe et al., 1997). In the soft-sphere model, the Newtonian equation of motion of individual particles was integrated. The collisions between particles and between particle and wall were simulated using Hooke's linear springs and dash pots (Cundall and Strack, 1979). This model has been used for investigating inter-particle force effect on fluidization characteristics (Kuwagi et al., 2000; Rhodes et al., 2001), mixing and segregation characteristics (Kaneko et al., 1999; Limtrakul et al., 2003), fluid dynamics (Rong et al., 1999), particle residence time (Wang and Rhodes, 2003), and minimum fluidization velocity (Kafui et al., 2002) in the bubbling fluidized bed. Kawaguchi et al. (1998) simulated particle motions in the spouted bed using the discrete element method (DEM). The DEM simulation has been used to investigate the mechanism of agglomeration in a fluidized bed of cohesive fine particles (Mikami et al., 1998; Kuwagi and Hoiro, 2002). On the other hand,

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the hard-sphere models are successfully used to model particle–particle and particle–wall collisions. The bubble formation and motions of particles in bubbling fluidized bed are investigated (e.g., Hoomans et al., 1996; Xu and Yu, 1997; Ouyang and Li, 1999; Helland et al., 2000; van Wachem et al., 2001). Goldschmidt et al. (2002) studied the particle velocity distributions and collision characteristics from dynamic discrete particle simulations in dense gas-fluidized beds. They found that for elastic particles the individual particle velocity function was an isotropic Maxwellian, and an anisotropic Maxwellian particle velocity distribution was observed for highly inelastic and rough particles. Recently, Tsuji et al. (1998) and Yuu et al. (2001) studied air and particle motions in a three-dimensional turbulent fluidized bed using the direct Monte Carlo simulation method (DMCS).

On the other hand Euler–Euler two-fluids models consider all phases to be continuous and fully interpenetrating. The equations employed are a generalization of the Navier–Stokes equations for interacting continua. Owing to the continuum representation of the particle phases, Eulerian models require additional closure laws to describe the rheology of particles. In most recent continuum models constitutive equations according to the kinetic theory of granular flow are incorporated. This provides explicit closures that take energy dissipation due to non-ideal particle–particle collisions into account by means of the coefficient of restitution. The models predicted well the bubble formation and the distribution of time-averaged solids concentration in bubbling fluidized beds (e.g., Ding and Gidaspow, 1990; Lyczkowsky et al., 1993; Kuipiers et al., 1993; Schmidt and Renz, 1999; Peirano et al., 2002). An isotropy of the particle velocity distribution is assumed in the kinetic theory of granular flow, which makes dense gas–solid fluidized beds questionable for two reasons: (1) The net action of all external forces in vertical direction will disturb isotropy of the particle velocity distribution, if particles are significantly accelerated between successive collisions. (2) It seems unlikely that all impact angles are of equal likelihood, which causes collisional anisotropy leading to anisotropic velocity distributions of particles (Goldschmidt et al., 2002).

The purpose of this paper is to simulate a detailed process of motion of particles in a bubbling fluidized bed using the hard-sphere discrete particle model. The particle motion consists of both collision and free flight steps. The particle interaction is described as instantaneous, binary, and inelastic collision with friction. The particle motion is controlled not only by gas-phase flow determining the flight step but also by action from its neighboring particles. The interaction forces between gas and particle obey Newton's third law. The gas-phase turbulent flow is modeled by a simple subgrid scale (SGS) model. The flow mechanism in a two-dimensional group-D particle bubbling fluidized bed is discussed. The particle pressure is calculated based on both the kinetic theory of granular flow and the normal stresses obtained from the simulated instantaneous particle velocity distributions. The radial distribution function is predicted based on the simulated spatio-temporal particle distributions. The simulation results are compared to the isotropic Maxwellian particle velocity distribution for the kinetic theory of granular flow. An agreement with the kinetic theory is obtained for elastic particles. The individual particle velocity distribution function is isotropic and Maxwellian. However, for inelastic particles an anisotropic Maxwellian velocity distribution is obtained. The observed anisotropy becomes more pronounced with increasing degree of inelasticity of the particles.

2. Eulerian–Lagrangian gas–solid flow model

2.1. Continuity and momentum equation for gas phase

The Eulerian–Lagrangian method computes the Navier–Stokes equation for the gas phase and the motion of individual particles by the Newtonian equations of motion. For the gas phase, we write the equations of conservation of mass and momentum as

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

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \mathbf{v}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot \tau_g + \varepsilon_g \rho_g \mathbf{g} - \sum_{i=1}^{N_p(v)} f_i. \tag{2}$$

The coupling term $\sum_{i=1}^{N_p(v)} f_i$ between the gas and the particle phase is estimated as the sum of the drag on each particle within the corresponding fluid control volume. The stress tensor of gas phase can be represented as

$$\boldsymbol{\tau}_g = \mu_g[\nabla \mathbf{v}_g + (\nabla \mathbf{v}_g)^{\mathrm{T}}] - \tfrac{2}{3}\mu_g(\nabla \cdot \mathbf{v}_g)\mathbf{I}. \tag{3}$$

The gas phase turbulence is modeled using a simple subgrid scale (SGS) model. The model was first used and proposed by Deardorff (1971) for channel turbulence flow. The SGS model simulates the local Reynolds stresses arising from the averaging process over the finite-difference grid by about the crudest of methods, that involve an eddy coefficient with magnitude limited in some way by the size of the averaging domain. This domain is considered to be the grid volume in a detailed numerical integration. Then the eddy coefficient becomes a "subgrid scale" coefficient.

$$\mu_g = \mu_{\mathrm{lam},g} + \rho_g (C_t \Delta)^2 \sqrt{S_g : S_g}, \tag{4}$$

where $\Delta = (\Delta x\, \Delta y)^{1/2}$ and $S_g = \frac{1}{2}[\nabla \cdot \mathbf{u}_g + \nabla \cdot \mathbf{u}_g^{\mathrm{T}}]$. Deardorff (1971) suggested C_t be in the range of 0.1–0.2. In this study $C_t = 0.1$ was used in the simulations.

2.2. Equations for the solid phase

Analysis of particle's collision in this study is based on collision dynamics with the following assumptions: (1)