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The effects of particle and gas properties on the fluidization of Geldart A particles

M. Ye, M.A. van der Hoef, J.A.M. Kuipers*

Fundamentals of Chemical Reaction Engineering, Faculty of Science and Technology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

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Abstract

We report on 3D computer simulations based on the soft-sphere discrete particle model (DPM) of Geldart A particles in a 3D gas-fluidized bed. The effects of particle and gas properties on the fluidization behavior of Geldart A particles are studied, with focus on the predictions of U_{mf} and U_{mb}, which are compared with the classical empirical correlations due to Abrahamsen and Geldart [1980. Powder Technology 26, 35–46]. It is found that the predicted minimum fluidization velocities are consistent with the correlation given by Abrahamsen and Geldart for all cases that we studied. The overshoot of the pressure drop near the minimum fluidization point is shown to be influenced by both particle–wall friction and the interparticle van der Waals forces. A qualitative agreement between the correlation and the simulation data for U_{mb} has been found for different particle–wall friction coefficients, interparticle van der Waals forces, particle densities, particle sizes, and gas densities. For fine particles with a diameter $d_p < 40\,\mu\text{m}$, a deviation has been found between the U_{mb} from simulation and the correlation. This may be due to the fact that the interparticle van der Waals forces are not incorporated in the simulations, where it is expected that they play an important role in this size range. The simulation results obtained for different gas viscosities, however, display a different trend when compared with the correlation. We found that with an increasing gas shear viscosity the U_{mb} experiences a minimum point near 2.0×10^{-5} Pa s, while in the correlation the minimum bubbling velocity decreases monotonously for increasing μ_g.

Keywords: Discrete particle simulation; Geldart A particles; Fluidized bed; Fluidization

1. Introduction

Geldart A particles are defined as *aeratable* particles, which normally have a small particle size ($d_p < 130\,\mu\text{m}$) and low particle density ($< 1400\,\text{kg/m}^3$). This kind of particles can be easily fluidized at ambient conditions (Geldart, 1973). The enormous relevance of the fluidization properties of Geldart A particles for industrial applications has long been recognized in chemical reaction engineering, in particular in the context of fluidized bed reactors containing FCC powders. A typical property of Geldart A particles is that they display an interval of non-bubbling expansion (homogeneous fluidization) between the minimum fluidization velocity U_{mf} and the minimum bubbling velocity U_{mb}, which is absent in the fluidization of large particles (Geldart B and D particles). It is precisely this homogeneous fluidization which is responsible for many unique features displayed by these reactors. Notwithstanding the intense experimental research that has been conducted in the past 30 years (Geldart, 1973; Abrahamsen and Geldart, 1980; Tsinontides and Jackson, 1993; Menon and Durian, 1997; Cody et al., 1999; Valverde et al., 2001), there is still no consensus on the precise mechanism underlying the homogeneous fluidization. Consequently, there exists currently no comprehensive theoretical approach, which is capable of describing both the homogeneous fluidization *and* bubbling behavior on the basis of gas and particle properties. Foscolo and Gibilaro (1984) suggested that the fluid–particle

* Corresponding author. Tel.: +31 53 489 3000; fax: +31 53 489 2479.
E-mail address: j.a.m.kuipers@ct.utwente.nl (J.A.M. Kuipers).

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interaction is the dominant factor that controls the stability of the homogeneous fluidization regime. On the other hand, Rietema and Piepers (1990) and Rietema et al. (1993) proposed that the interparticle forces are responsible for the homogeneous fluidization behavior of small particles. Although both viewpoints are partially supported by some experiments (Geldart, 1973; Abrahamsen and Geldart, 1980; Tsinontides and Jackson, 1993; Menon and Durian, 1997; Cody et al., 1999; Valverde et al., 2001) and theoretical work (Koch and Sangani, 1999; Buyevich, 1999; Buyevich and Kapbasov, 1999; Sergeev et al., 2004), a complete hydrodynamical description, based on either of them, is still not sufficient to model dense gas–solid flows involving Geldart A particles. This significantly limits the use of state-of-the-art CFD techniques in the design and scale-up of fluidized bed reactors with Geldart A particles.

Clearly, a detailed study of the particle–particle interactions and particle–fluid interaction at a more fundamental level is highly desirable. Discrete particle models (DPM) can play a valuable role in such studies. DPM has been widely used in the study of gas-fluidized beds, for example, the hard-sphere approach by Hoomans et al. (1996), Ouyang and Li (1998), and Zhou et al. (2002), and the soft-sphere approach by Tsuji et al. (1993), Xu and Yu (1997), Mikami et al. (1998), and Kafui et al. (2002). The idea of discrete particle simulation is to track the motion of each particle in the system by solving Newton's equations of motion. In DPM the details of the particle–particle (and particle–wall) collisions, including friction, can be readily incorporated. Furthermore, because of the *two-way coupling*, discrete particle simulations allows to study the influence of particle properties on the bed dynamics or vice versa (Li and Kuipers, 2003).

Recently, several attempts have been made (Kobayashi et al., 2002; Xu et al., 2002; Ye et al., 2004a) to study the fluidization behavior of Geldart A particles by use of 2D discrete particle simulations. Kobayashi et al. (2002) studied the effect of both the lubrication forces and the van der Waals forces on the relationship between pressure drop and the gas velocity for Geldart A particles. They showed the existence of a non-bubbling (homogeneous) regime, where it was found that both the cohesive and lubrication forces affected the profile of pressure drop for a decreasing gas velocity, but not for an increasing gas velocity. Xu et al. (2002) investigated the force structure in the homogeneous fluidization regime of Geldart A particles, where they found that the van der Waals forces acting on the particles are balanced by the contact forces. They also reported void structures during the "homogeneous" fluidization. In a previous 2D DPM study, we observed many of the typical features of Geldart A particles in gas-fluidized beds, such as the homogeneous expansion, gross particle circulation in the absence of bubbles, fast bubbles at fluidization velocities beyond U_{mb} (Ye et al., 2004a), and void structures (Ye et al., 2004b). An analysis of the velocity fluctuation of Geldart A particles suggests that homogeneous fluidization actually represents a transition phase resulting from the competition between three kinds of basic interactions: the fluid–particle interaction, the particle–particle collisions (and particle–wall collisions) and the interparticle van der Waals forces (Ye et al., 2004a,b). However, these DPM simulations were based on 2D geometries, and focused on the influence of cohesive forces on the flow patterns or flow structures. No modeling work has been carried out so far which studies the effect of the properties of both the particulate phase and gas phase on fluidization of Geldart A particles, although the classical empirical correlations (Abrahamsen and Geldart, 1980) have been proposed more than two decades ago. The main purpose of this paper is, for the first time, to make a comprehensive comparison with the well-known empirical correlation by Abrahamsen and Geldart, 1980 (in particular for U_{mf} and U_{mb}.), using a full 3D soft-sphere DPM to model the fluidization of Geldart A particles. In Section 2 the discrete particle model is briefly described. The details of the simulation procedure are discussed in Section 3, which is followed by a presentation of the simulation results. The paper ends with conclusions and a discussion.

2. Discrete particle model

In the discrete particle model, the gas-phase hydrodynamics is described by the volume-averaged Navier–stokes equations, following the approach of Kuipers et al. (1992).

$$\frac{\partial(\varepsilon\rho_g)}{\partial t} + (\nabla\cdot\varepsilon\rho_g\mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial(\varepsilon\rho_g\mathbf{u})}{\partial t} + (\nabla\cdot\varepsilon\rho_g\mathbf{u}\mathbf{u}) = -\varepsilon\nabla p - \mathbf{S}_p - \nabla\cdot(\varepsilon\overline{\tau}) + \varepsilon\rho_g\mathbf{g}. \tag{2}$$

No energy equations are considered in our model. This can be justified since we are studying the fluidization behavior at ambient conditions where it is anticipated that heat effects are small, so that the gas and particle flows can be safely assumed as isothermal. The gas flow is treated as compressible as the local gas pressure and density might be locally different. The gas phase flow field is computed on a Eulerian grid (with computational cell volume V) using the well-known SIMPLE algorithm (Patankar, 1980). The gas phase density ρ_g is calculated via the equation of state of an ideal gas law:

$$\rho_g = \frac{pM_g}{RT}, \tag{3}$$

where R is the universal gas constant $(8.314\,\mathrm{J/mol\,K})$, T the temperature, and M_g the molar mass of the gas. The equation of state of the ideal gas can be applied for most gases at ambient temperature and pressure. The coupling with the particulate phase is included by means of a source term $\mathbf{S}_p$, which is formally defined as

$$\mathbf{S}_p = \frac{1}{V}\int\sum\mathbf{F}_{\mathrm{drag},a}\,\delta(\mathbf{r}-\mathbf{r}_a)\,\mathrm{d}V, \tag{4}$$