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Validation of a discrete element model using magnetic resonance measurements

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ABSTRACT

The discrete element model (DEM) is a very promising modelling strategy for two-phase granular systems. However, owing to a lack of experimental measurements, validation of numerical simulations of two-phase granular systems is still an important issue. In this study, a small two-dimensional gas-fluidized bed was simulated using a discrete element model. The dimensions of the simulated bed were 44 mm × 10 mm × 120 mm and the fluidized particles had a diameter $d_p = 1.2$ mm and density $\rho_p = 1000\ \text{kg/m}^3$. The comparison between DEM simulations and experiments are performed on the basis of time-averaged voidage maps. The drag-law of Beetstra et al. [Beetstra, R., van der Hoef, M. A., & Kuipers, J. A. M. (2007b). *Drag force of intermediate Reynolds number flow past mono- and bidispersed arrays of spheres*. AIChE Journal, 53, 489–501] seems to give the best results. The simulations are fairly insensitive to the coefficient of restitution and the coefficient of friction as long as some route of energy dissipation during particle–particle and particle–wall contact is provided. Changing the boundary condition of the gas phase at the side-walls from zero-slip to full-slip does not affect the simulation results. Care is to be taken that the cell sizes are chosen so that a reasonable number of particles can be found in a fluid cell.

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1. Introduction

Gas-fluidized beds are widely used in industry; their applications range from drying, coating to fluid-catalytic cracking and gasification or combustion of carbonaceous fuels. However, despite their widespread use, the understanding of the underlying physics is still far from complete. Indeed, even single-phase granular systems, such as vibrating beds are still not fully understood.

Some understanding of the complicated underlying physics of two-phase granular phenomena such as bubble formation, coalescence or splitting may, however, be derived from numerical simulations. The two main approaches used to simulate gas–solid systems are the so-called two-fluid model, or Euler–Euler simulation and discrete element modelling. In discrete element modelling, each particle is treated as a single entity. Thus, polydispersity can be incorporated and there is no need for any expression for solid pressure and viscosity of the solid phase. The forces acting between colliding particles are given by contact mechanics, with the overall motion of each particle being governed by Newton's second law. The only closure required is the particle–fluid interaction, i.e. the drag-force. Various degrees of sophistication are possible in the contact mechanics; however, the impact of various contact models on the simulation of two-phase granular systems has yet to be investigated thoroughly.

However, a problem is experimental validation of discrete element models. Performing measurements in granular systems is inherently difficult as they are visually opaque. Traditionally, DEM simulations have mainly been validated by single-point measurements, such as pressure fluctuations or bed height. Some validation has been performed based on velocity measurements in 2D beds using particle image velocimetry (PIV) (Link, Cuypers, Deen, & Kuipers, 2005). A disadvantage of PIV is that measurements can only be performed close to the front wall of a two- dimensional fluidized bed. To our knowledge no comparison between experimental voidage measurements and DEM simulations has yet been performed. Several techniques to perform measurements in 3D granular systems exist, e.g. electrical capacitance tomography (ECT), X-ray tomography, diffusive wave scattering (DWS), positron emission particle tracking (PEPT) and magnetic resonance (MR). MR has the advantage that it can generally measure both velocities and voidages and has been applied in fluidized bed research to study mixing, the motion, formation, coalescence and eruption of bubbles and slugs and the velocity of the particulate phase (Müller et al., 2006; Müller, Davidson, et al., 2007; Müller, Holland, et al., 2007; Rees et al., 2006). Recently it has been shown by Holland, Müller, Dennis, Gladden, and Sederman (2008) that MR can be used

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Nomenclature

A	coefficient (–)
B	coefficient (–)
c	instantaneous hydrodynamic velocity (m/s)
C_D	drag coefficient (–)
d_p	particle diameter (m)
e	coefficient of restitution (–)
$\mathbf{F}_C$	contact forces (N)
$\mathbf{F}_p$	particle-fluid exchange (N/m^3)
g	gravity vector (m/s^2)
h	height above the distributor (m)
$\mathbf{I}$	identity matrix (–)
I_p	moment of inertia (kg m^2)
l	transverse thickness of the bed (m)
m_p	mass of a particle (kg)
p	pressure (Pa)
Re	Reynolds number (–)
t	time (s)
T_p	torque (kg m^2/s^2)
$\mathbf{u}$	fluid velocity (m/s)
U	fluidization velocity (m/s)
$\mathbf{v}_p$	particle velocity (m/s)
V	volume (m^3)
V_{cell}	volume of fluid cell (m^3)
V_p	volume of particle (m^3)
x; y; z	Cartesian coordinates (m)

Greek letters

β	momentum exchange coefficient (kg/(m^3 s))
ε	voidage (–)
λ	bulk viscosity (kg/(m s))
μ	shear viscosity (kg/(m s))
ρ	density (kg/m^3)
σ	coefficient of friction (–)
τ	viscous shear tensor (Pa)
Φ	constant (–)
χ	coefficient (–)
ω_p	rotational velocity (s^{-1})

to measure the mean collision time and the spatially resolved velocity fluctuations in 2D and 3D gas-fluidized beds, thus providing MR measurements of fluidized beds at very small time-scales, viz., of a few ms.

A discrete element model has some "flexibility" with respect to a few input parameters, such as the coefficient of restitution, coefficient of friction, drag law, boundary conditions at the wall, etc. Therefore, before numerical simulations, after validation by experimental measurements, can be used to understand the behaviour of real systems, the impact of these parameters on the simulated results needs to be understood. There has been some investigation, especially by Kuiper's group, of the influence of these parameters on the simulated results. For example, Beetstra, van der Hoef, and Kuipers (2007a) reported that the boundary condition of the gas phase at the side-walls of a two-dimensional fluidized bed had an appreciable influence on the segregation behaviour in a 2D fluidized bed. The influence of the coefficients of friction and restitution on the fluidization state was studied by Li and Kuipers (2007). It was found that bubbles only formed if some route for energy dissipation was provided, e.g. coefficient of restitution <1.0. Ye, van der Hoef, and Kuipers (2005) investigated the influence of the coefficient of friction and the gas boundary condition at the side-wall on the simulated results of a 2D fluidized bed of Geldart's Group A particles. They reported that the influence of the coefficient of friction was negligible on the predicted value of U_{mb}. However, the initial overshoot in pressure increased with increasing coefficient of friction. A change of the gas boundary condition from free-slip to zero-slip at the sidewalls had no effect on the predicted value of U_{mf}. Also, no effect was observed on the predicted pressure drop and expanded bed height. However, the predicted value of U_{mb} was higher if the zero-slip boundary condition was applied. Furthermore, the influence of the value of the Hamaker constant to describe the van der Waals (Ye et al., 2005) interaction between the Geldart's Group A particles was investigated. It was found that increasing the value of the Hamaker constant had no influence on the predicted value of U_{mf}, but led to an increase in U_{mb}. The influence of the Hamaker constant on the flow structure in 2D fluidized beds of Geldart A particles was also studied by Ye et al. (2005). It was reported that increasing the Hamaker constant led to a prolonged period of bed expansion. Kaneko, Shiojima, and Horio (1999) varied the stiffness of the spring, which represented the elastic part of the contact force in the normal direction, between 8 and 80,000 N/m but could visually not observe any difference during the start-up of the fluidized bed simulations.

In this paper, we report on the validation of a discrete element model by MR measurements of the time-averaged voidage in a small fluidized bed. The influence of simulation parameters, such as the coefficient of restitution, the drag law or the applied boundary conditions were studied and conclusions drawn as to their relative importance in the practical simulations of gas-fluidized beds.

2. Discrete element model

In this work, a two-phase discrete element model was constructed based on the work of Tsuji, Kawaguchi, and Tanaka (1993), which combined the discrete element model (DEM) of Cundall and Strack (1979) to simulate the particulate phase with the volume-averaged Navier–Stokes equations for the fluid phase, as derived by Anderson and Jackson (1967). For each particle, the linear and angular momenta are governed by Newton's 2nd law:

$$m_p \frac{d\mathbf{v}_p}{dt} = -V_p \nabla p + \frac{V_p \beta}{(1-\varepsilon)}(\mathbf{u} - \mathbf{v}_p) + m_p \mathbf{g} + \mathbf{F}_c, \quad (1)$$

$$I_p \frac{d\boldsymbol{\omega}_\mathbf{p}}{dt} = \mathbf{T}_p, \quad (2)$$

where m_p, $\mathbf{v}_p$, $\boldsymbol{\omega}_\mathbf{p}$, $\mathbf{u}$, β, $\mathbf{F}_C$, $\mathbf{T}_p$ and I_p are the mass, linear and angular velocity of the particle, the velocity of the gas phase, the interphase momentum exchange coefficient, the force and torque resulting from the collision of the particles and the moment of inertia of the particle, respectively. Our work was concerned with Geldart's Group B/D particles where interparticle forces are negligible. However, if systems of cohesive or small particles are to be simulated, additional forces, e.g. van der Waals forces, have to be considered. To model the collision between contacting particles the soft-sphere approach was used, in which the contact between particles is not assumed to be instantaneous. In the normal direction of the contact, the Hertzian contact model was applied, whereas in the tangential direction the contact model of Tsuji, Tanaka, and Ishida (1992) was used, whereby Coulomb's law is applied, i.e. if the tangential contact force exceeds a critical value sliding occurs. For the gas, the volume-averaged continuity and Navier–Stokes equations are given by Anderson and Jackson (1967):

$$\frac{\partial(\varepsilon \rho_f)}{\partial t} + \nabla \cdot (\varepsilon \rho_f \mathbf{u}) = 0, \quad (3)$$

$$\frac{\partial(\varepsilon \rho_f \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon \rho_f \mathbf{u}\mathbf{u}) = -\varepsilon \nabla p - \nabla \cdot (\varepsilon \boldsymbol{\tau}_\mathbf{f}) - \mathbf{F}_p + \varepsilon \rho_f \mathbf{g}, \quad (4)$$

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