Chemical Engineering Science 91 (2013) 1–4

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Note

Fully resolved simulation of a gas-fluidized bed: A critical test of DEM models

S.H.L. Kriebitzsch*, M.A. van der Hoef, J.A.M. Kuipers

Department of Chemical Engineering & Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands

HIGHLIGHTS

- Direct Numerical Simulation of gas-fluidized beds were done.
- The individual fluid–particle drag is compared with the force as evaluated in unresolved Discrete Element Models.
- The average DEM drag is found to be about 33% smaller than the "true" DNS drag.

ARTICLE INFO

Article history:
Received 14 May 2012
Received in revised form
6 December 2012
Accepted 20 December 2012
Available online 31 December 2012

Keywords:
Fluidization
Multiphase flow
Particle
Fluid mechanics
Direct numerical simulation
Gas–solid force

ABSTRACT

We performed Direct Numerical Simulation (DNS) of a gas-fluidized bed using the Immersed Boundary method combined with traditional Computational Fluid Dynamics. We have compared the individual fluid–particle force with the force as evaluated in an unresolved Discrete Element Model (DEM) simulation using closures for the gas–solid force for one fluidisation condition. We find that the average DEM gas–solid force is about 33% smaller than the "true" value which follows from the DNS model. For more realistic DEM simulations, a modification of the gas–solid force calculation is required, for instance by adding fluctuations or including the effect of the granular temperature.

1. Introduction

In the past 10 years, discrete elements models (DEMs) have become increasingly popular for modeling gas fluidized beds, and have now established themselves as a standard tool in the study of such systems (Deen et al., 2007) on a laboratory scale. A typical feature of discrete element models is that the flow is unresolved, that is, the gas phase is described on a scale larger than the size of the particles. As a consequence, the gas–solid interaction cannot be described at the scale of a single particle, but rather at the scale of the smallest computational unit of the gas-phase, i.e. a single computational fluid dynamics (CFD) cell. The gas–solid interaction force on a particle i with velocity $\mathbf{v}_i$ is then determined by the cell-averaged porosity ε and flow velocity $\mathbf{u}$, typically via a relation like

$$\mathbf{F}_{g,i}^{\mathrm{DEM}} = 3\pi\mu d\pi(\mathbf{u}-\mathbf{v}_i)\cdot F(\varepsilon,\mathrm{Re}_i), \quad \mathrm{Re} = \frac{\rho d\varepsilon|\mathbf{u}-\mathbf{v}_i|}{\mu}, \tag{1}$$

where F is a correlation that has to specified, d is the particle diameter (for simplicity we consider monodisperse systems), and μ and ρ are the viscosity and density of the gas phase, respectively. Note that it is common to evaluate the porosity and flow velocity at the location of particle, by an interpolation of the values of ε and $\mathbf{u}$ of all the cells within a certain range of the particle, so that the values depend slightly on the location of the particle (Deen et al., 2007). We stress that Eq. (1) is the total gas–solid interaction force, which can be split into a drag force and a pressure gradient force:

$$\mathbf{F}_g = \mathbf{F}_d - V_P\nabla p, \tag{2}$$

where V_P is the volume of the particle. We consider two correlations for $F(\varepsilon,\mathrm{Re})$: the combined Ergun and Wen and Yu correlation (see Gidaspow, 1994):

$$F(\varepsilon,\mathrm{Re}) = \begin{cases} \varepsilon^{-3.65}\left(1+0.15\mathrm{Re}^{0.687}\right) & \text{for } \varepsilon > 0.8, \\ \dfrac{150}{18}\dfrac{(1-\varepsilon)}{\varepsilon^2} + \dfrac{1.75}{18}\dfrac{\mathrm{Re}}{\varepsilon^2} & \text{for } \varepsilon < 0.8 \end{cases} \tag{3}$$

* Corresponding author. Tel.: +31 40 247 3666; fax: +31 40 247 5833.
E-mail addresses: S.H.L.Kriebitzsch@tue.nl (S.H.L. Kriebitzsch), M.A.v.d.Hoef@tue.nl (M.A. van der Hoef), J.A.M.Kuipers@tue.nl (J.A.M. Kuipers).

0009-2509/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ces.2012.12.038

and the correlation by Beetstra et al. (2007), obtained from lattice Boltzmann simulations (with $\phi = 1-\varepsilon$):

$$F(\varepsilon,\mathrm{Re}) = \frac{180}{18}\frac{\phi}{\varepsilon^2} + \varepsilon^2(1+1.5\phi^{1/2}) + \frac{0.413}{24}\left[\frac{\varepsilon^{-1}+3\varepsilon\phi+8.4\mathrm{Re}^{-0.343}}{1+10^{3\phi}\mathrm{Re}^{-(1+4\phi)/2}}\right]\frac{\mathrm{Re}}{\varepsilon^2}. \quad (4)$$

In this paper we want to put the current class of DEMs to the test, by performing a fully resolved simulation of a fluidized bed – which treats the gas–particle interaction *ab initio*. Since in such a simulation the "true" force on a particle is known at any moment in time, we can compare this with the gas–solid force that would have been evaluated for that particle in the framework of a DEM simulation using relations of the type (1). To our knowledge, this is the first fully resolved simulation of an actual gas-fluidized bed.

2. Simulation details

2.1. DNS method

For the solid phase, a simple hard sphere code is used, where the particle collisions are binary and instantaneous; the change in velocity and angular momentum due to the gas–solid force is calculated every CFD timestep. Note that this is different from DEM simulations, where only the change in *linear* momentum due to the gas–solid interaction is modelled. The gas flow field is obtained from the full Navier–Stokes equation using state-of-the art Computational Fluid Dynamics (CFD) methods, where a first-order-accurate method is used to discretize the momentum equations in time, in which the pressure, viscous and convective terms are treated implicit, semi-implicit and explicit, respectively. The no-slip boundary conditions at the surface of the particle are enforced by use of the Immersed Boundary (IB) method (Peskin, 2002); This is done by adding a force term $\boldsymbol{f}^{\mathrm{IB}}$ to the Navier–Stokes equations:

$$\rho_G\left(\frac{\partial}{\partial t}\boldsymbol{u} + \boldsymbol{\nabla}\cdot\boldsymbol{u}\boldsymbol{u}\right) = -\boldsymbol{\nabla}P + \mu\Delta\boldsymbol{u} + \boldsymbol{f}^{\mathrm{IB}}, \quad (5)$$

with fluid density ρ_G, fluid velocity $\boldsymbol{u}$, pressure P and dynamic viscosity μ.

The implementation that we adopt is along the lines of Uhlmann (2005). We have validated the code for a number of standard test cases, such as the hydrodynamics interaction force between two approaching spheres, and the hydrodynamic force for flow past regular and random arrays. Here only a brief outline of the method is given, details of the implementation and verification are published in Kriebitzsch (2011).

The basic idea is that the surface of the sphere is covered with markerpoints (see Fig. 1), each of which exerts a force on the fluid such that the gas-phase velocity is equal to the surface velocity at the location of the marker point, thereby modeling "no-slip" boundary conditions. The "essential" steps to compute the IB forcing term $\boldsymbol{f}^{\mathrm{IB}}$ are as follows:

- interpolation of fluid velocity to markerpoints m:
$$\boldsymbol{U}_m = \sum_{i,j,k} D(\boldsymbol{x}_{i,j,k}-\boldsymbol{X}_m)\cdot\boldsymbol{u}_{i,j,k} \quad (6)$$

- compute the force at the markerpoint as the difference of the current interpolated fluid velocity and the velocity of the particle at the location of the markerpoint:
$$\boldsymbol{F}_m^{IB} = \frac{\rho}{\Delta t}(\boldsymbol{V}_m-\boldsymbol{U}_m) \quad (7)$$

- mapping of force $\boldsymbol{F}^{\mathrm{IB}}$ back to the Eulerian grid:
$$\boldsymbol{f}_{i,j,k}^{IB} = \sum_m D(\boldsymbol{x}_{i,j,k}-\boldsymbol{X}_m)\cdot\boldsymbol{F}_m^{IB}\cdot\frac{\Delta V_m}{\delta^\beta} \quad (8)$$

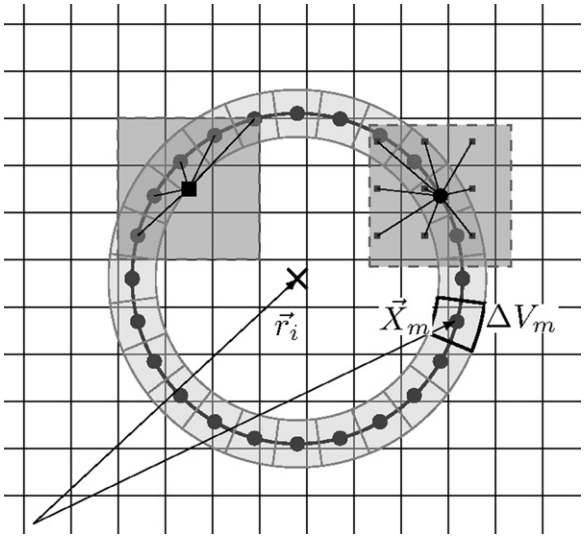

Fig. 1. The 2D sketch of an immersed object. The object is represented by a number of markerpoints, which are used to compute the force density $\boldsymbol{f}^{\mathrm{IB}}$.

$D(\boldsymbol{x}_{i,j,k}-\boldsymbol{X}_m)$ denotes a so-called discrete or regularized delta function with a finite support, which is computed as the product of one-dimensional regularized delta function. As indicated by the shaded squares in Fig. 1, we use a width of three Eulerian grid cells as support, hence in a $3\times3\times3$ cube in 3D.

The sum of the forces $\boldsymbol{F}^{\mathrm{IB}}$ from the markerpoint of one sphere i is equal to the total force that the sphere applies to the fluid, and hence the negative of this is $\mathbf{F}_{g,i}^{\mathrm{DNS}}$, which is used in the update of the position of the sphere.

2.2. Simulation settings

The physical properties of air are used for the density and dynamic viscosity of the gas phase: $\rho = 1.2$ kg/m^3, $\mu = 1.8\times10^{-5}$ Pa.s. The particle diameter d and particle density ρ_p are set to $d=1$ mm and $\rho_p = 1000$ kg/m^3, which in the Geldart classification this corresponds to B-type particles. The timestep to update the gas flow was set to $\delta t = 1\times10^{-5}$ s, while the gridsize δl was set to $d/10$. Choosing a coarser grid (i.e. $d/6.5$) did not influence the results. We performed simulation of a gas-fluidized bed of 2000 particles, with a width equal to $W=14.8$, $d=14.8$ mm, a depth $D=5.6$, $d=5.6$ mm, and a height $H=42$ mm; the height of the bed in the packed state was 21.2 mm. The bed was fluidized with a superficial velocity $U_o = 0.5$ m/s, which is roughly two times the minimum fluidization velocity. The typical particle Reynolds number at this velocity is $\mathrm{Re} = \rho d U_o/\mu = 35.3$. Constant pressure outflow boundary condition was used at the top, and no-slip boundary conditions were used on all side walls. In the simulations, relatively homogeneous fluidisation was observed with a wave-like expansion behaviour of the particle bed that means the bedheight fluctuates periodically (see also Verloop and Heertjes, 1974). The average bed height in the fluidized state was 29.0 mm, and the corresponding porosity was 0.563. For comparison, we have also run a DEM simulation of the same system; the timestep was the same as in the DNS and the grid size was about $3d$. We found that the bedheight was significantly lower in that case (26.2 mm), and also the characteristics of the bed oscillations was different. Snapshots from both simulations are shown in Fig. 2.

3. Comparisons with DEM type gas–solid force models

One of the assets of DNSs is that the actual (or "true") gas–solid force on each individual particle is known at any point in