Particuology xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Particuology

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

Modeling particle sedimentation in viscous fluids with a coupled immersed boundary method and discrete element method

Sayed M. Derakhshani [a,b,*], Dingena L. Schott [a], Gabriel Lodewijks [a]

[a] Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Delft, Netherlands
[b] Department of Mechanical Engineering, Faculty of Engineering, University of Isfahan, Isfahan, Iran

ARTICLE INFO

Article history:
Received 11 November 2015
Received in revised form 14 July 2016
Accepted 21 September 2016
Available online xxx

Keywords:
Immersed boundary method
Discrete element method
Particle sedimentation
Boycott phenomenon

ABSTRACT

Numerical techniques have increasingly been used to model fluid–particle two-phase flows. Coupling the immersed boundary method (IBM) and discrete element method (DEM) is one promising approach for modeling particulate flows. In this study, IBM was coupled with DEM to improve the reliability and accuracy of IBM for determining the positions of particles during the sedimentation process within viscous fluids. The required ratio of the particle diameter to the grid size (D/dx) was determined by comparing the simulation results with the analytical solution and experimental data. A dynamic mesh refinement model was utilised in the IBM model to refine the computational fluid dynamics grid near the particles. In addition, an optimum coupling interval between the IBM and DEM models was determined based on the experimental results of a single particle sedimentation within silicon oil at a Reynolds number of 1.5. The experimental results and the analytical solution were then utilised to validate the IBM–DEM model at Reynolds numbers of 4.1, 11.6, and 31.9. Finally, the validated model was utilised to investigate the sedimentation process for more than one particle by modeling the drafting-kissing-tumbling process and the Boycott phenomenon. Benchmark tests showed that the IBM–DEM technique preserves the advantages of DEM for tracking a group of particles, while the IBM provides a reliable and accurate approach for modeling the particle–fluid interaction.

Introduction

Multiphase flow is a simultaneous flow of materials with different states or phases (i.e., gas, liquid, or solid) or materials with different chemical properties in the same state or phase (Brennen, 2009). Multiphase flow has been extensively researched owing to its importance and application in industrial and natural processes. Particle transportation within fluids appears in processes associated with filtration, dust emission, pharmaceutical applications, and the food industry (Eshghinejadfard, Abdelsamie, Janiga, & Thévenin, 2016). A quantitative understanding of the micro-scale phenomena of fluid–particle interactions could facilitate the establishment of general methods for reliable scale-up, design, and control of particulate systems and processes (Derakhshani, Schott, & Lodewijks, 2015; Zhao & Shan, 2013). Combining the Lagrangian and Eulerian approaches can be used to capture the microscopic information at the particle level relevant to the fluid–particle interactions. The discrete element method (DEM) is used to model the inter-particle interactions and the collisions between particles and the domain wall. The fluid flow can be fully solved around the particle phase with the immersed boundary method (IBM). Combining the IBM and DEM methods has computational efficiency and effort advantages over other coupling approaches, such as the Lattice–Boltzmann DEM (LB–DEM) and the direct numerical simulation DEM (DNS–DEM) (Gao & Sun, 2011).

In this study, open-source packages are employed to model the coupling between the particle phase and fluid flow. LIGGGHTS (Kloss, Goniva, Hager, Amberger, & Pirker, 2012) is used to model the particles, OpenFOAM (www.openfoam.com) is used to model the fluid flow, and CFDEM (Goniva, Kloss, Aichinger, & Pirker, 2009) is used to couple the DEM and IBM models. The numerical accuracy should be carefully considered in the selection of the numerical method and software. Hence, the IBM–DEM model is first checked for reliability and accuracy by modeling a single particle sedimentation (SPS) problem. The validated model is then utilised to model the drafting-kissing-tumbling (DKT) process (Fortes, Joseph, & Lundgren, 1987) and the Boycott phenomenon (Boycott, 1920).

---

* Corresponding author at: Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Delft, Netherlands.
E-mail address: s.m.derakhshani@tudelft.nl (S.M. Derakhshani).

http://dx.doi.org/10.1016/j.partic.2016.09.006
1674-2001/© 2017 Chinese Society of Particuology and Institute of Process Engineering, Chinese Academy of Sciences. Published by Elsevier B.V. All rights reserved.

Nomenclature

D	Diameter (mm)
F	Force (N)
g	Gravitational acceleration (m/s^2)
h, H	Height (mm)
I	Moment of inertia (kg m^2)
k	Stiffness constant (N/m)
L	Length (mm)
m	Mass (kg)
p	Pressure (Pa)
R	Radius (mm)
t	Time (s)
T	Torque (kg m/s^2)
u	Velocity (m/s)
V	Volume (m^3)
W	Width (mm)

Greek

γ	Viscoelastic damping constant (N s/m)
δ	Overlap displacement (m)
ε	Void fraction
μ	Dynamic viscosity (Pa s)
ν	Poisson's ratio
ρ	Density (kg/m^3)
τ	Shear stress (N/m^2)
ω	Angular velocity (rad/s)

Subscripts

f	Fluid
n	Normal
p	Particle
t	Tangential

SPS is a simplified case of a multi-phase flow problem in which the behavior of a single spherical particle in the fluid flow is studied. In this study, the physics of the SPS problem, such as the flow regime, driving and damping forces, and the level of their influence on the accuracy of the numerical solution is evaluated by comparison with analytical solutions and reliable experimental data. Choosing a suitable temporal discretization scheme and the optimum coupling interval are the other aims of this study. These parameters are calibrated according to experimental data of a single particle settling within silicon oil (ten Cate, Nieuwstad, Derksen, & Van den Akker, 2002). In addition, the optimum ratio of the particle diameter to the computational fluid dynamics (CFD) grid size (D/dx) and the local refinement value of the CFD cells are determined to accurately simulate the particle sedimentation based on the analytical results and experimental data.

The validated IBM–DEM model is then used to simulate the DKT process and the Boycott phenomenon. The DKT process is the simplest situation involving more than one particle. When two particles located with one above the other sediment in a closed container within a viscous fluid, the DKT process occurs between them (Shao, Liu, & Yu, 2005). The DKT phenomenon has been studied by a number of researchers (Breugem, 2012; Derakhshani, Schott, & Lodewijks, 2016; Eshghinejadfard et al., 2016; Glowinski, Pan, Hesla, Joseph, & Périaux, 2001; Sharma & Patankar, 2005). In this study, the simulation results of the IBM–DEM model are compared with the IBM results of Breugem (2012) and the LB–IBM results of Eshghinejadfard et al. (2016). In the 1920s, Boycott (1920) observed that the settling behavior of blood cells within an inclined test tube is much faster than in a vertical tube. The sedimentation of a pack of 50 particles within a cuboid is modeled to reproduce the Boycott effect within an enclosure filled with a viscous fluid. In the SPS and DKT case studies, the main role of the DEM model was the determination of the precise position of the particle phase in the CFD domain. In the Boycott phenomenon, the interactions between particles and the particle–wall collisions are of importance and are studied in detail for different tube inclination angles. The results of this research will be employed in future research modeling the dust liberation phenomenon.

Theoretical framework

This section provides the theoretical description of the analytical and numerical models that are utilised to model particle sedimentation within a fluid. In Section Analytical formulation of SPS, the analytical model of the particle sedimentation within the fluid is described in detail. The governing equations of the fluid flow along with a description of the DEM contact model are presented in Sections Governing equations of the fluid phase and Discrete element method (DEM), respectively. The coupling method between the IBM and DEM models is explained in Section IBM–DEM technique.

Analytical formulation of SPS

The trajectory and terminal velocity of a spherical particle during the sedimentation process can be determined analytically in order to be used as a criterion for evaluating the accuracy of a numerical model. The forces involved in the SPS phenomenon are categorised into driving forces and damping forces. In the SPS problem, the only driving force is the gravity force (F_g), which forces a particle to settle downward through the fluid. The damping forces including the buoyancy force (F_b), drag force (F_d), virtual mass force (F_vm), Basset force (F_Basset), and lift forces act in the opposite direction of gravity. Considering the above-mentioned forces, the momentum equation for the particle is as follows:

$$\left(m_\mathrm{p} + C_\mathrm{A}\rho_\mathrm{f}V_\mathrm{p}\right)\frac{du_\mathrm{p}}{dt} = gV_\mathrm{p}\left(\rho_\mathrm{p} - \rho_\mathrm{f}\right) - \frac{1}{8}\pi C_\mathrm{D}{D_\mathrm{p}}^2\rho_\mathrm{f}{u_\mathrm{p}}^2$$

$$-C_\mathrm{H}{D_\mathrm{p}}^2\sqrt{\pi\rho_\mathrm{f}\mu_\mathrm{f}}\int_0^t \frac{\partial u_\mathrm{p}}{\partial t\prime}/\sqrt{t - t\prime}dt\prime, \tag{1}$$

where C_A and C_H are the added mass and history term coefficients, respectively, which can be determined from experimental data (Odar & Hamilton, 1964). D_p, V_p, ρ_p, and u_p are the diameter, volume, density, and velocity of the particle, respectively, and ρ_f and μ_f are the density and dynamic viscosity of the fluid, respectively.

The SPS consists of three stages: acceleration, steady speed (terminal velocity), and deceleration. Each stage is influenced by different forces. For instance, the Basset and virtual mass forces play an important role in the acceleration stage while they have a negligible effect in the other stages (Bagherzadeh, 2014). In addition, the lubrication force is unavoidable when a particle gets close enough to the boundaries of a domain. It is possible to calculate these forces in the numerical model and analytical formulation in order to make comparisons.

Governing equations of the fluid phase

The momentum equation of the fluid phase within a porous medium along with the conservation of mass is presented in this section. The continuity equation of the fluid phase is given by

$$\frac{\partial\left(\varepsilon_\mathrm{f}\rho_\mathrm{f}\right)}{\partial t} + \nabla\cdot\left(\varepsilon_\mathrm{f}\rho_\mathrm{f}\mathbf{u}_\mathrm{f}\right) = 0, \tag{2}$$

Please cite this article in press as: Derakhshani, S. M., et al. Modeling particle sedimentation in viscous fluids with a coupled immersed boundary method and discrete element method. *Particuology* (2017), http://dx.doi.org/10.1016/j.partic.2016.09.006