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SIMULATION OF PARTICLE-WALL COLLISIONS IN A VISCOUS FLUID USING A RESOLVED DISCRETE PARTICLE METHOD

Zhi-Gang Feng

Department of Mechanical Engineering University of Texas at San Antonio San Antonio, TX79258, USA zhigang.feng@gmail.com

Efstathis E. Michaelides Department of Mechanical Engineering University of Texas at San Antonio San Antonio, TX78258, USA <u>Stathis.michaelides@utsa.edu</u> Shaolin Mao T-5, Theoretical Division Los Alamos National Laboratory Los Alamos, NM 87545, USA <u>smao@lanl.gov</u>

ABSTRACT

The process of particle-wall collisions is very important in understanding and determining the fluid-particle behavior, especially near walls. Detailed information on particle-wall collisions can provide insight on the formulation of appropriate boundary conditions of the particulate phases in two-fluid models. We have developed a three-dimensional Resolved Discrete Particle Method (RDPM) that is capable of meaningfully handling particle-wall collisions in a viscous fluid. This numerical method makes use of a Finite-Difference method in combination with the Immersed Boundary (IB) method for treating the particulate phase. A regular Eulerian grid is used to solve the modified momentum equations in the entire flow region. In the region that is occupied by the solid particles, a second particle-based Lagrangian grid is used, and a force density function is introduced to represent the momentum interactions between particle and fluid. We have used this numerical method to study both the central and oblique impact of a spherical particle with a wall in a viscous fluid. The particles are allowed to move in the fluid until they collide with the solid wall. The collision force on the particle is modeled by a soft-sphere collision scheme with a linear spring-dashpot system. The hydrodynamic force on the particle is solved directly from the RDPM. By following the trajectories of a particle, we investigate the effect of the collision model parameters to the dynamics of a particle close to the wall. We report in this paper the rebound velocity of the particle, the coefficient of restitution, and the particle slip velocity at the wall when a variety of different soft-sphere collision parameters are used.

INTRODUCTION

Inter-particle and wall collisions are very important in particle-fluid flows. The dynamic behavior of such flows is decided by these collisions, especially when the flow is dense and the particles move at high velocity. Particulate flow modeling, as an effective and robust tool to study many issues associated with particular flows (segregation, agglomeration, and clustering), requires the ability of accurately resolving inter-particle and wall collisions. The correct handling of these collisions is an essential element for the discrete particle method (DPM) or discrete element method (DEM), which will not work without an accurate knowledge of the collisions. Therefore, an artificial mechanism is necessary to be introduced in the numerical simulation to account for the collision force during collision processes. Without such a mechanism in the model, it is likely that the particles will penetrate significantly into each other's computational boundary, thus, rendering the results meaningless. Some commonly used collision schemes include the hard-sphere scheme [1], the repulsive force scheme [2], and the soft-sphere scheme [3]. The soft-sphere collision scheme, as the most popular one, requires several pre-defined collision parameters;

however, how to choose these parameters is still an unsolved problem [4].

There are a few experimental studies on the particleparticle and particle-wall collision in a viscous fluid. Joseph et al. [5, 6] presented data for the coefficient of restitution of a spherical particle when it strikes a vertical wall in a viscous, stagnant fluid. They studied both central and oblique impacts using particles of different materials. The rebound of a falling particle that impacts a submerged surface has also been studied by Gondret et al. [7]. Zhang et al. [8] studied experimentally the collision of a falling sphere with a stationary sphere in a viscous fluid. They also studied numerically the collision with a numerical technique based on the lattice Boltzmann method. On the analytical side, Jenkins and Louge [9] considered the granular flow of hard colliding spheres bounded by a flat frictionless wall. Benyahia et al. [10] demonstrated that the behavior and the collisions of particles at the walls play an important role in the predictions of two-fluid models. Ardekani and Rangel [11] numerically investigated the dependence of the coefficient of restitution on the Stokes number and surface rougheness.

In this paper we study the collision of a sphere with a solid wall in a viscous fluid. The sphere is given an initial velocity; it is allowed to travel through the viscous fluid and then strikes a solid wall obliquely and rebounds from it. We use a three-dimensional RDPM in combination with a collision model to study the motion of the sphere before and after the collision. The collision force is modeled by the softsphere scheme with a linear-dashpot model [12]. The effects of the collision parameters to the particle dynamics is investigated by comparing the rebound velocity of the particle and the slip velocity on the wall. The paper is organized as follows: first we briefly describe the immersed boundary based RDPM and the soft-sphere collision scheme that are used in the present study; then we provide some numerical simulations results of the oblique impact of a particle with a wall; results are also compared with experimental data found in literature.

PROBLEM DESCRIPTION

IB based RDPM

Combined with direct forcing scheme [13], the IB [14] based DNS has been implemented successfully to solve particle and fluid momentum interactions by Feng and Michaelides [15], and Uhluman [16]. Here, we present a brief description of this method. Consider a particulate flow system composed of circular rigid particles suspended in the two-dimensional incompressible Newtonian fluid, as shown in Figure 1. The entire computational domain, Ω is composed of the fluid region, *L*, and the solid particle region, $\sum S_i (S_I + S_2)$ in the figure). The domain is surrounded by a boundary, Γ . The boundary or surface of the *i*-th particle S_i is denoted by ∂S_i



Figure 1: Conceptual model of two circular particles suspended in a fluid.

Based on the concept of IB and the direct-forcing scheme, the fluid field for the entire domain Ω which is occupied by the fluid and the solid particles, can be described by using the following set of dimensionless governing equations:

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \vec{\nabla} \vec{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \vec{u} + \vec{f}, \quad \vec{x} \in \Omega$$
(1)

where \vec{u} and p are the dimensionless fluid velocity and pressure, \vec{f} is the force density accounts the presence of solid boundary in fluid, Re is the flow Reynolds number.

B. For the force density field:

$$\vec{f} = \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} + \nabla p - \frac{1}{\text{Re}} \nabla^2 \vec{u}, \quad \vec{x} \in \sum S_i$$
(2)

C. Continuity equation:

$$\vec{\nabla} \cdot \vec{u} = 0, \quad \vec{x} \in \Omega \tag{3}$$

D. For the velocity field inside a solid particle region:

$$\vec{u} = \vec{U}_i + \vec{\omega}_i \times (\vec{x} - \vec{x}_i) \tag{4}$$

Here, \vec{x}_i is the center of the *i*-th particle; \vec{U}_i and $\vec{\omega}_i$ are the translational and angular velocities of the particle, respectively.

E. For the motion of the particles:

$$(\rho_r - 1)V_p \frac{d\vec{v}_i}{dt} = \int \vec{f} \, dV + (\rho_r - 1)V_p \vec{g} + \vec{F}_i^{col} \tag{5}$$

$$\frac{l_p}{\rho_r}(\rho_r - 1)\frac{d\overline{\omega}_i}{dt} = -\int (\vec{x} - \vec{x}_i) \times \vec{f} \, dV + \vec{T}_i^{col} \tag{6}$$

where ρ_r is the particle-fluid density ratio, V_p and I_p are the volume of a particle and its moment of inertia; \vec{F}_i^{col} and \vec{T}_i^{col} are the resultant force and moment on the *i*-th particle caused by particle-particle and particle-wall collisions.

The above set of equations, together with boundary conditions and initial conditions, is solved numerically using finite-difference based scheme, as detailed in our previous paper [17,18].

The soft-sphere collision scheme

The prescription of a definitive collision scheme is necessary for any discrete particle method. There are several collision schemes available in the literature. The so-called "soft-sphere scheme" with a linear spring-dashpot system is the most popular one and it will be studied here. The particlewall collision may be considered as special cases of the interparticle collision when the radius of one of the particle approaches infinity. The contact forces, which are composed by the normal and tangential forces, are evaluated from the overlapping displacement and their relative velocities. Using the linear spring-dashpot model, the normal contact force is:

$$f_{ij}^{\ n} = -k_n \delta^n_{\ ij} - \eta_n v^n_{\ ij} \tag{7}$$

where δ_{ij}^n is the normal overlapping displacement, k_n and η_n are the normal spring stiffness and damping coefficient, and v_{ij}^n is the relative normal velocity component (particle *j* with respect to particle *i*). Where δ_n is the overlap normal displacement component, $(v_p)_n$ is the particle velocity component in the normal direction of the wall. The tangential collision force is given by:

$$f_{ij}^{\ t} = -k_t \delta^t_{\ ij} - \eta_t v^t_{\ ij} \tag{8}$$

where δ_{ij}^t is the tangential overlapping displacement; k_t and η_t are the tangential spring stiffness and damping coefficient respectively; and v_{ij}^t is the relative tangential velocity component at the contact point which can be computed as follows:

 $\vec{v}_{ij}^t = \vec{v}_{ij} - (\vec{v}_{ij} \cdot \hat{n}_{ij})\hat{n}_{ij} + [\vec{\omega}_i \times r_i \vec{n}_{ij} - \vec{\omega}_j \times r_j (-\vec{n}_{ij})]$ (9) When one considers the friction at contact, the tangential contact force can be calculated from the expression:

$$f_{ij}{}^{t} = \begin{cases} -k\delta^{t}{}_{ij} - \eta v^{t}{}_{ij}, & if \ |f_{ij}{}^{t}| \le \mu_{s}|f_{ij}{}^{t}| \\ \mu_{k}|f_{ij}{}^{t}|\frac{\delta^{t}{}_{ij}}{|\delta^{t}{}_{ij}|}, & if \ |f_{ij}{}^{t}| > \mu_{s}|f_{ij}{}^{t}| \end{cases}$$
(10)

where μ_s , and μ_k are the coefficients of static and dynamics friction, respectively. However, most studies do not differentiate between μ_s and μ_k and use a single coefficient of friction, μ . The slider distance or tangential displacement can be computed by integrating the relative tangential velocity within the contact time.

In the soft-sphere model, there are five model parameters need be specified: the spring stiffnesses in the normal and tangential springs; the damping coefficients for the normal and tangential dashpots; and the coefficient of friction. The normal spring stiffness for dry collisions has been well studied both theoretically [19] and experimentally [20]. It is determined by the material properties of the particles. Spring stiffnesses ranging from 200,000 dyn/cm (200 N/m) to 50,000,000 dyn/cm (50,000 N/m) have been used in the modeling of solidgas flows [12, 21]. The use of small spring stiffness allows a larger time step to be used in the simulation. However, a softer spring may cause significantly particle-particle overlapping. Little is known on the choice of model parameters for particle-wall and particle-particle collisions in a viscous fluid. In our simulation the spring constant k is chosen between 250,000 dyn/cm and 2,000,000 dyn/cm; the damping coefficient is chosen between 0 and 100 dyn.s/m (0.1 N.s/m).

RESULTS AND DISCUSSIONS

We studied the collision of a sphere with a solid wall. Figure 2 shows the schematic diagram of a sphere approaching a solid wall with velocity \vec{v}_p at an angle, θ . The sphere has a diameter *d* and it is instantaneously located at a distance *L*, from the wall. A $\theta = \frac{\pi}{2}$ will correspond to a central impact.



Figure 2: A schematic diagram of a sphere moving towards a wall at velocity V_p and incident angle of θ .

Comparison simulation results with experimental study

Joseph et al. [5] measured coefficient of restitution e for the central particle-wall collisions both in air and water. They found e=0.98 when it is in air and e=0.8 when it is in water. This indicates that the collision in air can be considered as elastic impact and the viso-elastic effect during collision is insignificant. We consider the case of central particle-wall impact in water and use RDPM to simulate the collision.



Figure 3: Particle approaching and rebounding velocities during collision. Soft-sphere model with k=500,000 dyn/cm and e=0 are used

The particle-wall collisions are modeled by the softsphere model. The fluid field is solved by the RDPM. In the present study, we set d=0.635cm, L=1.5d, and θ =90°. The sphere has a density of 2.54 g/cm³ and the fluid has the properties of water, with ρ =1 g/cm³, and μ =0.01g/(cm.s). The particle velocity vector is approximately $v_p = 12$ cm/s horizontally after an initial short transition, yielding a Reynolds number of 762. The gravitational force is not included in the simulation. The physical box used in the simulations of the particle-wall collision is $2\text{cm}\times 2\text{cm}\times 4\text{cm}$. The results presented in this section are obtained using a uniform grid of $80\times 80\times 160$ with a time step equal to 5×10^{-6} s. To model an elastic impact, we set damping coefficient to be zero, and choose spring stiffness k to be 500,000 dyn.s/cm.

We compare our simulation results with the experimental measurement from Joseph et al. [5] in Figure 3. We have set t=0 as the time where the sphere is at L=1.5d away from the wall, instead of the beginning of particle-wall contact. Good agreement is found between the results modeled by the soft-sphere model and those experimental measured. The particle velocity is about 10.5 cm/s right before the impact; and its rebounding velocity is found to be 8.2 cm/s, which yields a coefficient of restitution e=0.78.

A finer grid with smaller grid spacing dx=0.02cm and time step ($dt=2.5 \times 10^{-6}$ s) is also used for the simulation and no significant difference between the results of these two grids is observed, as seen in Figure 3.

Effect of collision parameters to particle-wall impact

We study how the input parameters for the soft-sphere collision scheme affect the RDPM simulation results. We consider the oblique particle-wall impact by setting θ =45°. The physical properties of particle and fluid are the same as described previously. The particle velocity vector is approximately $\vec{v}_p = 12\vec{i} + 12\vec{j}$ cm/s at t=0.0005s which creates a particle diameter based Reynolds number of 1077. Here, \vec{i} and \vec{j} are the unit vectors in the horizontal direction and vertical directions, respectively.



Figure 4: particle velocity components before and after the collision at different spring constant with $\eta{=}50$ dyn.s/cm.

During the collision the viscous drag force on the sphere is computed directly through the resolved fluid field. The collision force is modeled by the soft-sphere collision model, which uses the five parameters that were enumerated above. We assumed the coefficient of friction to be $\mu = 0.3$; the spring stiffness k parameter to range from 250,000 dyn/cm to 2,000,000 dyn/cm; the damping coefficient η to be in the

range between 0 dyn.s/cm and 100 dyn.s/cm. The same spring stiffnesses and damping coefficients were used for both the normal and the tangential force components.

Figure 4 shows the normal velocity component (u) and tangential velocity component (w) of the particle before and after the collision process with four different spring stiffnesses; the damping coefficient was constant $\eta=50$ dyn.s/cm in all these cases. We observe that, in the normal direction the particle's rebound velocity is very close in all the cases with the normal coefficient of restitution being approximately 0.65. However, the increase of spring stiffness reduces the reduction of the tangential velocity component, which is due to the collision of the particles. The drop of the tangential velocity component is equal to the slip velocity at the wall during the collision process. This observation is very significant for the collision process and for the modeling of the solid phase boundary conditions because it implies that the no-slip velocity condition at the boundary is not a valid assumption for particle phase during collisions with a wall. Another important observation is that the collision duration is very much influenced by the choice of the spring stiffness. As the spring becomes softer and the spring stiffness decreases, the particle-wall contact time during the collision process increases.



Figure 5: Particle normal and tangential velocity components before and after the collision with different damping coefficients

Figure 5 shows the normal and tangential velocity components before and after the collision with the damping coefficient as a parameter and with the spring stiffness constant and equal to 1,000,000 dyn/cm. It is observed that, when the coefficient of damping is increased, the normal coefficient of restitution decreases. In the figure the coefficient of restitution drops from 0.76 at η =0 to 0.54 at η =100 dyn.s/cm. Also, when the coefficient of damping is increased the slip velocity also increases. The particle-wall contact time appears to be independent of the damping coefficient.

CONCLUSIONS

We numerically simulated the collision process of a solid sphere with a solid wall in a viscous fluid using an Immersed Boundary technique based Resolved Discrete Particle Method. The collision force on the particle is modeled by a soft-sphere scheme and is parameterized by two spring stiffnesses, two damping coefficients and one coefficient of friction. It is observed that the numerical scheme supplemented with the soft-sphere model describes the collision process accurately and determines a slip velocity for the particle. The slip velocity and the rebound velocity depend highly on the choice of the collision parameters. All the findings of this study point to the fact that the choice of the collision parameters for the collision scheme employed in the discrete particle method modeling is critical to the accurate simulation of particulate flows. Also, that during collisions there may be significant particle tangential slip at the wall, which must be accounted for in the boundary conditions of two-fluid models.

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REFERENCES

1. Hoomans, B.P.B.; J.A.M. Kuipers, W.J. Briels and W.P.M. van Swaaij, "Discrete particle simulation of bubble and slug formation in two-dimensional gas-fluidised beds: a hard-sphere approach," *Chem. Engng Sci.*, **51**:99 (1996).

2. Glowinski, R.; T.-W. Pan, T. I. Hesla, D. D. Joseph, and J. Periaux, "A fictitious domain approach to the direct numerical simulation of incompressible viscous flow past moving rigid bodies: application to particulate flow," *J. Comput. Phys.*, **169**: 363–426 (2001).

3. Tsuji, Y.; Y. Morikawa, T. Tanaka, N. Nakatsukasa, and N. Nakatani, "Numerical simulation of gas-solid two-phase flow in a two-dimensional horizontal channel," *Int. J. Multiphase Flow*, **13**:671 (1987).

4. Di Renzo, A and Di Maio, F.P., "Comparison of contactforce models for the simulation of collisions in DEM-based granular flow codes," *Chemical Engineering Science*, **59**:525-541 (2004).

5. Joseph, G. G.; R. Zenit, R., M. L. Hunt, and A. M. Rosenwinkel, "Particle-wall collisions in a viscous fluid," *J. Fluid Mech.*, **433**:329-346 (2001)

6. Joseph, G. G. and M. L. Hunt, "Oblique particle-wall collisions in a viscous fluid," *J. Fluid Mech.*, **510**:71-93 (2004).

7. Gondret, P.; M. Lance, & L. Petit, "Bouncing motion of spherical particles in fluids," *Phys. Fluids*, **14**:643-652 (2002).

8. Zhang, J.; L.-S. Fan, C. Zhu, R. Pfeffer, and D. Qi, "Dynamic behavior of collision of elastic spheres in viscous fluids," *Powder Technol.*, **106**:98-109 (1999)

9. Jenkins, J. T. and Louge, M. Y., "On the flux of fluctuation energy in a collisional grain flow at a flat, frictional wall," *Phys. Fluids*, **10**, 1836-1840, (1997).

10. Benyahiaa, S., Syamlala, M., and O'Brien, T.J., "Evaluation of boundary conditions used to model dilute, turbulent gas/solids flows in a pipe," *Powder Techn.*, **156**, 62-72, (2005).

11. A. M. Ardekani and R. H. Rrangel, "Numerical investigation of particle–particle and particle–wall collisions in a viscous fluid," *J. Fluid Mech.*, **596**:437-466 (2008).

12. Tsuji, Y.; T. Kawaguchi, and T. Tanaka, "Discrete particle simulation of two dimensional fluidized bed," *Powder Technol.* **77**:79.(1993).

13. Mohd-Yusof, J., "Combined immersed boundaries/B-splines methods for simulations of flows in complex geometries," *Annual Research Briefs*, Center for Turbulence Research, Stanford University (1997).

14. Peskin, C.S., "Numerical analysis of blood flow in the heart," *J. Comput. Phys.* **25**, 220–252 (1977).

15. Feng, Z.-G. and E. E. Michaelides, "Proteus: A direct forcing method in the simulations of particulate flow," *J. Comput. Phys.*, **202**: 20-51 (2005).

16. Uhlmann, M., "An immersed boundary method with direct forcing for the simulation of particulate flows," *J. Comput. Phys.*, **209**: 448-476 (2005).

17. Feng, Z-G, and Michaelides, E. E., "Inclusion of Heat Transfer Computations for Particle Laden Flows," *Physics of Fluids*, **20**:675-684 (2008).

18. Feng, Z.-G. and E. E. Michaelides, "Heat transfer in particulate flows with direct numerical simulation (DNS)," *Int. J. Heat Mass Transfer*, **52**:777-787 (2009).

19 . Johnson, K.L., *Contact Mechanics*, Cambridge University Press, Cambridge, UK (1985).

20. Mullier, M.; U. Tüzün, U. and O. R. Walton, "A singleparticle friction cell for measuring contact frictional properties of granular materials," *Powder Technol.* **65**:61 (1991).

21. Xu, B.H. and A. B. Yu, "Numerical simulation of the gassolid flow in a fluidized bed by combining discrete particle method with computational fluid dynamics," *Chem. Engng Sci.* **52**: 2785 (1997).