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Fully resolved binary particle interactions in isotropic turbulence using hard and soft sphere collision models

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Abstract – Binary particle collisions are studied using hard and soft sphere collision models in both stagnant and homogeneous isotropic turbulence boxes. Particle-fluid coupling was achieved using a ghost-cell immersed boundary method coupled with the spectral element method-based direct numerical simulation solver, Nek5000. The turbulent box was obtained using a stochastic forcing technique with a Reynolds number ($Re_\lambda \approx 2.5$) based on the Taylor microscale chosen to represent the viscous sublayer in a $Re_\tau = 180$ channel flow. Results indicate similar collision behaviour using the two models within both stagnant and turbulent fluids, with the hard sphere model predicting slightly less agglomeration compared with the soft sphere approach.

1. Introduction

Particle-laden flows refer to a type of multiphase system in which a particulate phase is distributed throughout a continuous fluid phase. Examples of such flows include aerosol delivery through spray medication, evaporation of milk droplets in spray driers and the separation of particles from air in industrial cyclones. The present work is of significance in the nuclear industry, where the decommissioning of legacy pond and silo wastes presents a major challenge. These wastes contain large inventories of particulate material, including corrosion products from magnesium-based alloy clad uranium metal (Magnox) fuel elements. Agglomeration of such particles during waste transport can result in deposition and blockages of pipes and pumps and fouling of process equipment. Improved understanding of the fundamental dynamics of particle interactions within these flows will allow for safer and more efficient decommissioning processes through manipulation of agglomeration behaviour.

The combination of direct numerical simulation for continuous phase modelling with particle-resolved methods such as the immersed boundary method (IBM) for discrete phase modelling, allows for high fidelity simulation of binary particle interactions. Within any discrete phase model, the collision dynamics are typically described using either a hard sphere or a soft sphere approach. Hard sphere models use conservation of momentum and energy to update the particle velocities post-collision and typically incorporate a coefficient of restitution to account for the inelastic component in particle deformation and friction to account for sliding and dissipation of energy during the collision. In contrast, the soft sphere model accounts for deformation of the particle upon collision by allowing the two spheres to overlap, where the repulsive force is proportional to the overlap distance. To do this, continuous treatment for unsteady particle deformation is applied throughout the interaction using small time-steps and discretised equations for the inter-particle stresses and contact mechanics. This makes it more computationally demanding than the alternative hard sphere approach but provides a more realistic description of the collision interaction.

Extensive studies utilise these models, but rarely have the two been actively compared in the context of agglomeration, particularly in fluid flow regimes. The aim of this work is therefore to produce a collision detection and resolution algorithm comparison between hard and soft sphere collisions. This will generate insight into the accuracy of the hard sphere method when compared to the soft sphere approach, allowing for more pragmatic models for simulating binary collisions to be developed. The particle collisions are studied in a stagnant box, and a box of homogeneous isotropic turbulence representing the viscous sublayer region of a $Re_\tau = 180$ channel flow, with particle properties matching those of calcite in water.

2. Methodology

Collisions were performed in dimensional cubic boxes with length 1mm, consisting of a mesh that is discretised equally into 20^3 smaller cubic spectral elements. Each of these elements are further discretised into 7 equivalent Gauss-Legendre-Lobatto nodes, meaning that the box contains around 2.7 million grid points. Spherical particles are represented by a computational icospherical mesh with 320 faces. Hydrodynamic forces are exerted on the particle by the fluid. The magnitude of these forces depends on the magnitude of the velocity fluctuations caused by turbulent eddies. Advection and rotation are applied to the particle by determining the local fluid pressure and viscous stress tensor and evaluating a translational force vector, as well as torque, with orientation solved for using the quaternion formulation. The interactions between the discrete and continuous phase are described by the ghost-cell based immersed boundary method developed by Mark and van Wachem (2008) which calculates and exchanges data simultaneously with the fluid-phase solver each time step.

The stability of a dispersion and thus its tendency to aggregate is ultimately dependent on the particle-particle interactions present. The magnitude of these interactions is described by Derjaguin, Landau, Verwey and Overbeek (DLVO) theory, an approach to model both the van der Waals and electrical double layer forces together to dictate the degree of attraction or repulsion two particles experience during a collision.

For the hard sphere model (Yamamoto et al. 2001), post-collision velocity components and positions are calculated each time step using a coefficient of restitution to account for energy dissipation during the collision:

$$\tilde{\boldsymbol{v}}_{p,i} = \boldsymbol{v}_{p,i} + \frac{(1+e)}{2}\Big((\boldsymbol{v}_{p,j} - \boldsymbol{v}_{p,i}) \cdot \hat{\boldsymbol{n}}\Big)\hat{\boldsymbol{n}} \tag{1}$$

$$\tilde{\boldsymbol{x}}_{p,i} = \boldsymbol{x}_{p,j} + \tilde{\boldsymbol{v}}_{p,i} t_{col} \tag{2}$$

Here, $\tilde{v}_p$ and v_p are the post- and pre-collision velocity components, respectively, with i and j labelling a pair of interacting particles, e is the normal coefficient of restitution and $\hat{\boldsymbol{n}}$ is the unit normal vector along the line joining particles i and j. Likewise, $\tilde{x}_p$ and x_p are the post- and pre-collision positions and t_{col} the collision time.

In contrast, the soft sphere model applies a 'soft sphere force' which includes normal contact behaviour described by Hertzian theory and a normal damping force. The additional force term for soft sphere collisions is presented in Eq. 3. Here $\boldsymbol{F}_{SSC}$ represents the soft sphere force, k_n the elastic coefficient, $\delta_{i,j}$ the intersection distance, η the damping coefficient and $\boldsymbol{u}_r$ the relative collision velocity vector:

$$\boldsymbol{F}_{SSC} = -k_n \delta_{i,j} \hat{\boldsymbol{n}} - \eta(\boldsymbol{v}_r \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}} \tag{3}$$

3. Results and Discussion

By injecting the particles into a stagnant box with no turbulence, the agglomeration behaviour simulated purely by the two collision models could be studied. The initial separation distance was selected to be just greater than the region where DLVO forces become important, whilst also ensuring a collision took place. For high initial velocities, particles were found to bounce, whilst at low velocities (0.175 mms^{-1} in Fig. 1) agglomeration was observed. For initial particle velocities far away from the transition region where particle agglomeration starts to occur, there was a strong agreement between the two collision models. However, approaching this region, discrepancies between the two models sharply increased in magnitude, with more kinetic energy lost during the soft sphere collisions as opposed to in the hard sphere collisions.

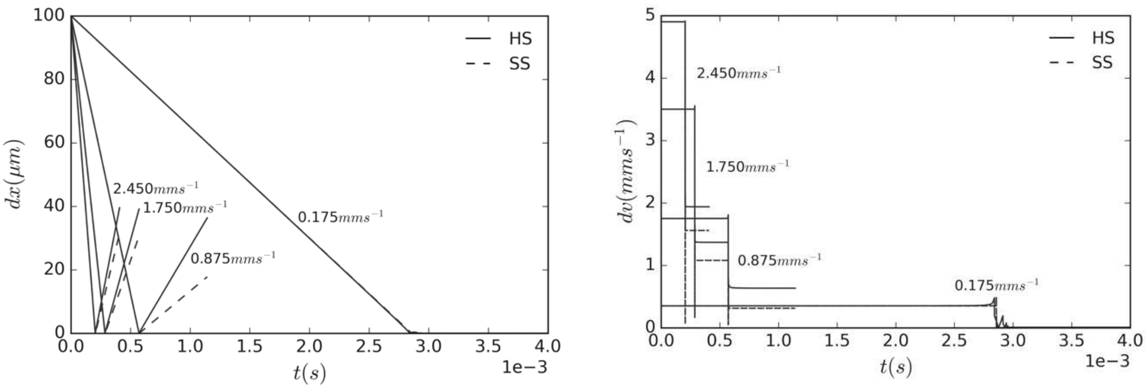

Figure 1: Temporal evolution of inter-particle separation distance (left) and relative velocity (right) for hard and soft sphere binary collisions in a stagnant box.

Studies by Mortimer et al. (2020) showed that most collisions within a channel flow occur within the viscous sublayer region due to increased particle velocity (${v_P}'_{rms}$) fluctuations within this region. The authors found that the fluid velocity fluctuations (v'_{rms}) within the viscous sublayer region to be ~0.05 ms^{-1}. The present work aims to augment this work, simulating a box with a Taylor Reynolds number (Re_λ) at a value typical of that region. Here, we use the agglomeration/bounce crossover region from the stagnant results as the mean relative collision velocities observed in the viscous sublayer region of the channel flow for the turbulent box. An average between the hard and soft sphere models of 0.007 ms^{-1} was used. Homogeneous isotropic turbulence was established by a stochastic forcing method following

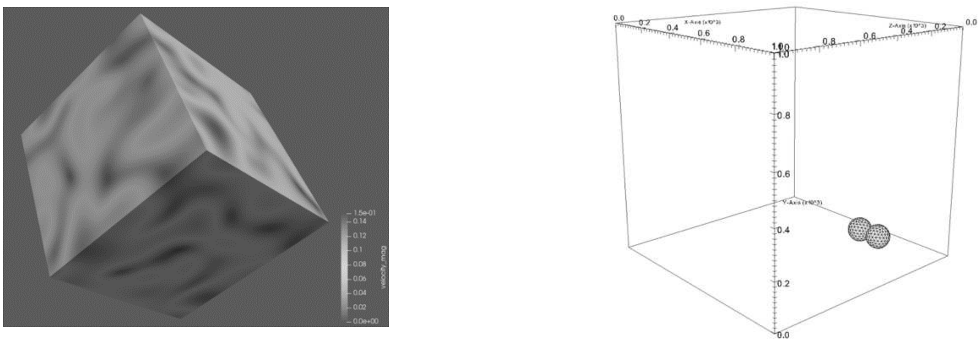

Figure 2 Velocity magnitude in isotropic turbulence (left) showing surface eddies and example of the random injection position of two particles inside the domain (right).

the method of Eswaran and Pope (1988). Parameters were selected to recreate the Re_λ and v'_{rms} values found in the viscous sublayer, demonstrated in Fig. 2.

Particles were injected at random positions within the turbulent box with an inter-particle separation of 5 μm to ensure a collision event occurred and to reduce computational time. Probability density functions from 45 particle collision simulations, see Fig. 3, were constructed to show the most likely outcomes. Results show similar predictions for both models, though particles modelled using the hard sphere model have a greater tendency to be closer together than the soft sphere approach, suggesting more agglomeration. These results conform to those found in the stagnant box.

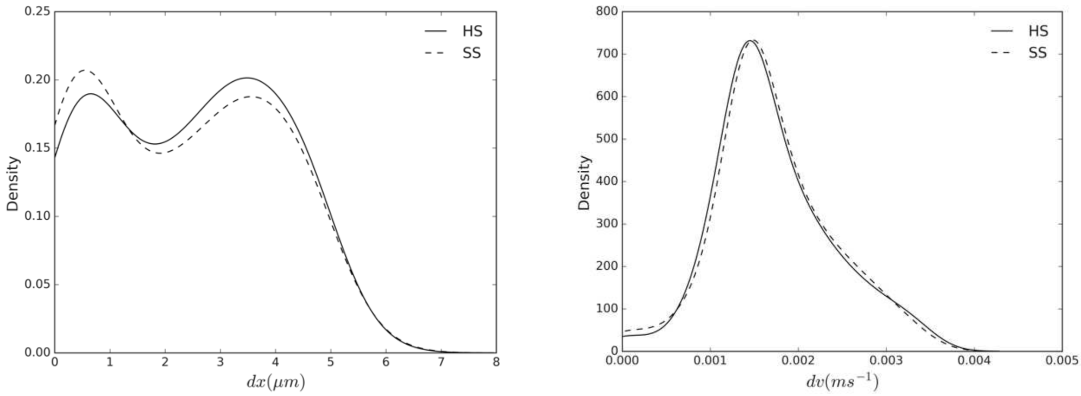

Figure 3: Probability density function of inter-particle separation (left) and relative velocity (right) produced from 45 particle collision simulations at 5 μm initial separation.

4. Conclusions

An IBM has been coupled with a fluid solver to predict binary particle interactions using hard and soft sphere collision models. When injected into a stagnant box, there were clear discrepancies between the two models, increasing as the agglomeration/bounce transition region was approached. This demonstrates a clear relationship between the collision model and particles agglomeration behaviour. A homogeneous box of isotropic turbulence was established, with properties matching those observed in the viscous sublayer of a channel flow. Due to the chaotic nature of the turbulence simulation, probability distribution functions have been produced across many sample collision events to determine the most likely outcomes of the two models. The results suggest less agglomeration when using the hard sphere model compared with the soft, which agrees with the results of the stagnant box simulations.

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