Agglomeration and collision behaviour of non-spherical particles in turbulence

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Abstract – Non-spherical particle-particle interactions are studied in detail under the influence of a fully resolved turbulent flow field and particle-fluid coupling scheme, which are obtained through direct numerical simulation and an immersed boundary method, the latter of which has been adapted to include particle agglomeration and non-sphericity. Agglomeration outcomes are successfully observed through the incorporation of attractive van der Waals forces under the DLVO framework, which is suitably adapted to consider the orientational dependencies associated with non-spherical shapes. Binary interactions take place in a periodic box of homogeneous, isotropic turbulence, which are maintained using a stochastic forcing method. The turbulence properties of the box have been matched to those observed in the viscous sublayer of a shear Reynolds $Re_\tau = 180$ channel flow. Differences in particle interaction behaviours are presented for the case of disks and needles in the periodic box. The roles of orientation and velocity in determining interaction outcomes are also assessed. Results indicate that the inclusion of DLVO forces promotes alignment between the symmetry axes of spheroidal particle pairs.

1. Introduction

The interaction behaviour of micron-scale particles in turbulence is relevant in many industrial settings. One important example is found in the nuclear industry, where legacy nuclear waste is kept in storage ponds awaiting transport to more sustainable long-term storage locations. During this interim period, and during transport, particles can collide together and form agglomerates. This poses a risk, since larger particles are more likely to deposit, potentially leading to pipe blockages which are expensive to rectify. A deeper understanding of such processes is therefore of great value to improved process and equipment design.

Agglomeration can be modelled through the inclusion of attractive van der Waals (vdW) forces. Consideration of the balance between these forces and the repulsive electric double layer (EDL) force in a liquid medium is covered by Derjaguin, Landau, Verwey and Overbeek (DLVO) theory. The combination of these two effects gives rise to a potential which is a function of the intersurfacial distance. In order to agglomerate, a pair of approaching particles must first have sufficient kinetic energy to overcome the potential barrier arising from the EDL force. Beyond this barrier, as the particles move closer still, there lies an attractive potential well. If the post-collision kinetic energy is too low for the particles to escape this well, then they remain bond and an agglomerate is formed. The majority of the studies of such particle interactions focus on spheres. However, particles found in real industrial systems will very often be non-spherical. Spheres are chosen for their mathematical simplicity but the effect of morphology is consequently poorly understood. Spheroids provide the opportunity to study needle- and disk-like particles of a desired aspect ratio.

The inclusion of turbulence to a particulate system leads naturally to the realisation of many interesting phenomena due to the wide range of interaction velocities and orientations being sampled in any given simulation. It has been observed that agglomeration rates differ across regions of a channel flow, owing to the different turbulence properties found in the different flow regions (Mortimer et al. 2020). Periodic boxes of isotropic turbulence provide the opportunity to recreate these turbulence properties but in a much smaller simulation domain, and hence a more computationally efficient way. In these small but representative regions of turbulence, the interplay between turbulence and particle agglomeration may be studied.

2. Methodology

The fluid-phase is computed through direct numerical simulation of the incompressible Navier-Stokes equations using the spectral element solver, Nek5000. The cubic domain encloses 20^3 evenly-spaced elements of seventh-order equating to 2.7 million grid points. The domain is $1\ mm$ in length, with periodic boundary conditions enforced. Turbulence is sustained within the domain through the use of a stochastic forcing function developed by Eswaran and Pope (1988). Six independent Uhlenbeck-Ornstein random processes are used to generate the forcing independently of the computed velocity field. The forcing is parameterised *a priori* such that the flow field converges upon a desired turbulence level. This is performed in Fourier-space, where only small wavenumbers, corresponding to the largest motions of the flow, are excited. The smaller-scale motions are formed through the natural turbulence energy cascade.

An immersed boundary method is utilised to couple the particle-phase to the fluid, where a no-slip condition is enforced at the particle-fluid interface using the ghost-cell mirroring technique (Mark and van Wachem 2008). The particle mesh is an icosphere consisting of 320 triangular faces, scaled to obtain a specific aspect ratio for non-spherical particles. Three different morphologies are represented using this approach, corresponding to a sphere, needle and disk. The radius of the sphere is chosen to be 50 μm and the volume is fixed across all morphologies. The advection and rotation of the particles are computed by considering the total hydrodynamic forces and torques acting at the particle surface. Non-spherical hard-sphere collisions are computed through an adaptation of the method of Jain et al. (2019) which also provides a means to compute the closest distance vector between spheroidal surfaces.

Due to their very short-range nature, most of the contribution to the DLVO force occurs around the point of nearest approach and different relative orientations lead to different geometric properties at this point. Everaers and Ejtehadi (2008) proposed a term $\chi_{ij}\eta_{ij}$ that accounts for the orientational dependency at this point based upon the local surface curvature. In the present work, this term is applied to give the following equation for the force between two interacting particles, where the first term on the RHS represents the vdW attraction and the second term describes the EDL repulsion:

$$\boldsymbol{F}_{DLVO} = -\chi_{ij}\eta_{ij}\left(\frac{Ar}{12|\boldsymbol{d}|^2} - \frac{64\pi r n k_B T \Theta^2 e^{-\kappa|\boldsymbol{d}|}}{\kappa}\right)\hat{\boldsymbol{d}}, \tag{1}$$

where $\boldsymbol{d}$ is the vector of closest approach, A is the Hamaker constant, r is the spherical radius, n is the number density of electrolyte ions, Θ is the reduced surface potential, k_B is the Boltzmann constant, T is the fluid temperature, and κ is the inverse Debye length. This force is evaluated at every timestep between particle pairs and is included in the force balance. The charge distribution is assumed to be uniform across the particle surface, in line with Hamaker theory.

3. Results and Discussion

A statistically stationary box of homogeneous and isotropic turbulence was simulated with properties representative of the viscous sublayer in a shear Reynolds number $Re_\tau = 180$ channel flow. As a particle pair moves with the mean channel flow, the relative collision velocity mostly arises due to the velocity components acting perpendicular to the mean flow, since the velocities experienced in the streamwise direction are similar. Hence, the velocities in the spanwise and wall-normal directions were used to determine the required Reynolds number based on the Taylor microscale ($Re_\lambda \approx 2.5$).

Pairs of disks and needles with aspect ratio 5:1 were then injected into the turbulent box at uniformly random positions, with a fixed minimal separation distance of 1 μm, as illustrated in Fig. 1. This distance was chosen to ensure that a collision occurred, but also to ensure the particles were outside of the effective range of the DLVO forces so that the full interaction was simulated. The particles were given an initial relative velocity of 0.0042 ms^{-1} which corresponds to the measured averaged collision velocity in the viscous sublayer of the channel flow. The chemical parameters were chosen to match calcite particles in water, used as a nuclear waste simulant. The interactions were allowed to run for 3 *ms*, which was enough time for the turbulence to significantly influence the particle velocities or for an agglomerate to form. Figure 2 highlights three key cases of interacting disks in the turbulent box. Case 1 is an example of an agglomerate forming. The method through which this occurs is energy loss in successive collisions reducing the relative velocities of the particles enough that they cannot escape the potential well by the final collision. In the second case, we observe the particles remaining close but not through an agglomeration event. Rather, the particles experience similar flow conditions due to being advected by the same turbulent eddy, and a small van der Waals contribution keeps them close before finally they are swept apart by an adverse velocity gradient. In the third case, the disks collide on their edges and hence the van der Waals force is not strong enough to greatly influence the collision at the given velocities and so they move apart indefinitely.

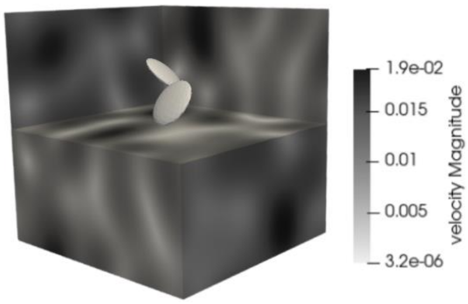

Figure 1: A pair of interacting disks in a turbulent velocity field ($Re_\lambda = 2.5$).

To understand which orientations lead to agglomeration in turbulence, and hence the kind of structures most likely to form, data was collected on the angles between the symmetry axes of disks and needles and compared in cases with and without agglomeration. Here we present 50 needle-needle simulations in which 25 particle pairs agglomerated and 25 did not. This led to the probability density functions given in Fig. 3. It can be observed that the particle pairs which agglomerate tended to have their symmetry axes aligned. The alignment of their symmetry axes facilitates the chance of an interaction taking place for which the surface interaction, and hence van der Waals forces, are maximal. Then, agglomeration is much more favourable. We see that the present background turbulence field is not strong enough to break agglomerates, but this is facilitated under the DLVO potential model.

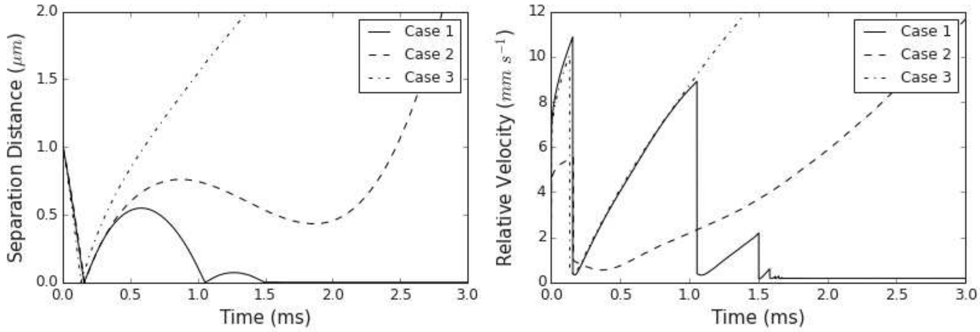

Figure 2: Temporal evolution of separation distance and relative velocity of three illustrative interaction cases between disks.

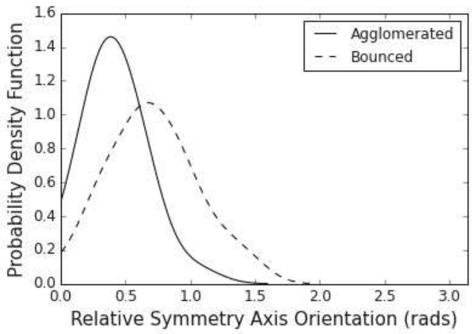

Figure 3: PDF of relative angle between particle symmetry axes for needles in the turbulent box compared for agglomerating and rebounding particles.

4. Conclusions

A methodology for the simulation and analysis of non-spherical particle interactions in turbulence has been demonstrated. Interactions of disks and needles in the viscous sublayer have been presented in demonstrative examples, where they have been analysed and the important features relating to agglomeration discussed. Resolution of non-spherical particle agglomeration has been achieved and it is shown that needles are more likely to agglomerate when their symmetry axes are aligned, such that their long axes are parallel to one another. The full paper includes a comparison of behaviours between three morphologies. Interaction behaviours are also contrasted between the turbulent flow case and a stagnant flow field.

References

L.F. Mortimer, D.O. Njobuenwu and M. Fairweather. Agglomeration dynamics in liquid-solid particle-laden turbulent channel flows using an energy-based deterministic approach. *Phys. Fluids*, 32: 043301, 2020.

V. Eswaran and S. B. Pope. An examination of forcing in direct numerical simulations of turbulence. *Comp. Fluids*, 16: 257-278, 1988.

A. Mark and B.G.M. van Wachem. Derivation and validation of a novel implicit second-order accurate immersed boundary method. *J. Comp. Phys.*, 227: 6660-6680, 2008.

R. Jain, S. Tschisgale, and J. Fröhlich . A collision model for DNS with ellipsoidal particles in viscous fluid. *Int. J. Multiphase Flow*, 120: 103087, 2019.

R. Everaers and M.R. Ejtehadi. Interaction potentials for soft and hard ellipsoids. *Phys. Rev. E*, 67: 041710, 2003.