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Direct numerical simulations of collision efficiency of cohesive sediments

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ABSTRACT

A clear understanding of the collision efficiency of cohesive sediment particles is critical for more accurate simulation of the flocculation processes. It is difficult, if not impossible, to carry out laboratory experiments to determine the collision efficiency for small particles. Direct Numerical Simulation (DNS) is a relatively feasible approach to describe the motion of spherical particles under gravity in calm water, and thus, to study the collision efficiency of these particles. In this study, the Lattice Boltzmann (LB) method is used to calculate the relative trajectories of two approaching particles with different ratios of sizes and densities. Results show that the inter-molecular forces (i.e., van der Waals attractive force, electrostatic repulsive/attractive force, and displacement force), which are usually neglected in previous studies, would affect the trajectories, and thus, lead to an overestimation of the collision efficiency. It is found that to increase the particle size ratio from 0.1 to 0.8 only slightly increases the collision efficiency, since the force caused by fluid-solid interaction between these two particles is reduced. To increase the submerged particle density ratio from 1 to 22, however, would significantly decrease the collision efficiency. Earlier analytical formulations of collision efficiency, which only consider the effects of particle size ratio, have significantly overestimated the collision efficiency (change from 0.01 to 0.6) when the particle size ratio is around 0.5.

1. Introduction

Flocculation/aggregation of colloidal particles is an important, but not well-understood process. Because of flocculation/aggregation, small colloidal particles, such as clay minerals (size < 2 μm), will form much larger flocs (varying in sizes from 10 to 1000 μm, depending on composition, ambient turbulence, salinity, or biological factors) that can easily settle on the seafloor (Manning and Dyer, 1999; Safak et al., 2013). The flocculation/aggregation process is not limited to pure clay particles, and flocs can be formed as a mixture of clay, silt, and/or organic matters. The presence of contaminants, e.g., heavy metal ions, can also change the flocculation rate. Flocculation/aggregation will significantly increase the settling velocity (w_s) of fine, cohesive sediments. Currently the capabilities of modeling w_s are still poor and need great improvements by better understanding the motions of fine, cohesive sediments in estuaries or many other water bodies. The above descriptions point to the need of more studies on flocculation/aggregation process, which is essential to improve the current capability of modeling cohesive sediment transport processes.

Two parameters are determining the aggregation process of cohesive particles. The first parameter, collision frequency (β_{ij}), or encounter rate (Hill et al., 1990), is defined as the count of collisions of one sphere with radius R_i collides with another sphere with radius R_j over a specified time period in a fluid. In calculating the collision frequency, only the trajectories of two far-away particles are used to determine whether they will collide or not. If the minimum distance of these two trajectories, x_c, is less than $R_i + R_j$, then there will be a collision (Friedlander, 1977). It is understood that to mimic the collision frequency, many particles (the number depending on the concentration of the particles) should be used to study the effect of turbulence and the possible collisions among particles. In this study, nevertheless, the main objective is to explore the collision efficiency of two approaching particles.

When two solid particles are getting closer, the intermolecular forces, i.e., the expelling/attractive electrostatic force, the van der

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Waals force, and the displacement force, become important, and these forces will affect their trajectories. This leads to adding another parameter, collision efficiency, E_{ij}, to work together with collision frequency for describing a collision event. Here the displacement force (caused by the fluid that is squeezed out when two particles are close) has been called "lubrication force" before (Kim and Karrila, 1991), but the name "displacement force" better describes the nature of this force, and thus, is used in this study.

Stolzenbach and Elimelich (1994) defined the collision efficiency as "the ratio of actual collisions to those that would occur if the larger particle collided with all the slower-sinking particles in the volume swept out by its cross-section as it sinks." Mazzolani et al. (1998) expressed the collision efficiency as $E_{ij} = x_c^2/(R_i + R_j)^2$, where x_c is the minimum distance/offset between these two parallel vertical lines that go through the centers of the two spheres, and R_i and R_j are the radii of these two spheres. Previous studies on this subject showed that one only needs to study the change of the relative trajectories of two particles to address their collision efficiency (Wacholder and Sather, 1974; Han and Lawler, 1991).

Although the concept of collision efficiency of cohesive sediments has been documented for around four decades (e.g., Hahn and Stumm, 1970; Pruppacher and Klett, 1978), Wacholder and Sather (1974) presented the first analytical solution of collision efficiency for two particles with different sizes (R_i and R_j) and different densities (ρ_i and ρ_j) falling in a calm fluid. They suggested that four regions can be identified on a chart that uses the ratio of their radii ($R_r = R_i/R_j$) and the ratio of their settling velocities ($w_r = R_r^2\Delta\rho_r$) as the two coordinates and the ratio of their submerged density ($\Delta\rho_r = (\rho_i - \rho_w)/(\rho_j - \rho_w)$) as a parameter to decide the collision efficiency. Region 1 ($0 \le \Delta\rho_r < \Delta\rho_{cr1}$): here $\Delta\rho_{cr1}$ is a function of R_r and it is the first critical value of $\Delta\rho_r$ to draw the border among regions (Fig. 1). In this region, if the original offset is larger than the critical offset, x_c, the relative trajectory will be deflected, i.e. small particle goes around the large particle and continues to move up, i.e., no collision. On the other hand, if the small particle is sufficiently close to the centerline, i.e., $x < x_c$, then it will collide with the large particle. Region 2 ($\Delta\rho_{cr1} \le \Delta\rho_r < \Delta\rho_{cr2}$): here $\Delta\rho_{cr2}$ is the second critical value of $\Delta\rho_r$ to draw the next border

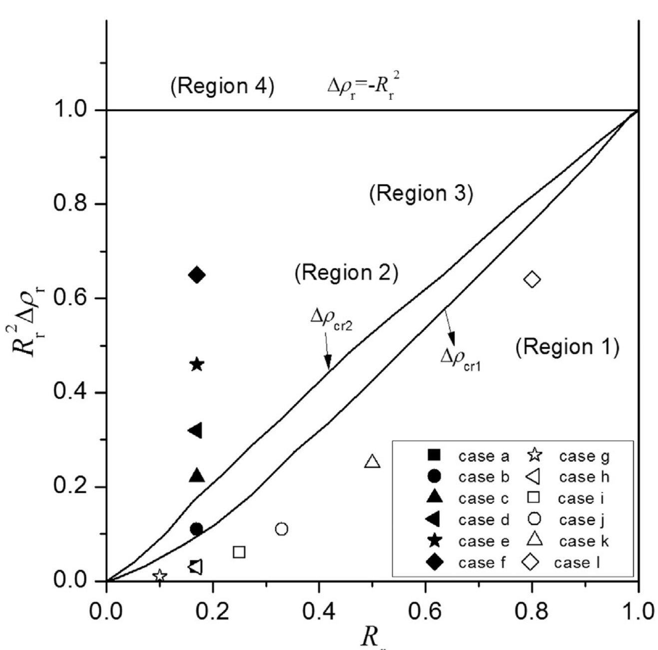

Fig. 1. Schematic plot of four different regions based on the critical ratio of density of two particles (Wacholder and Sather, 1974) used to decide the collision efficiency.

which may be approximated by a straight line $\Delta\rho_r\ R_r = 1$ for simplicity. Within this region, there are two possible trajectories. If the original offset, x, is less than a critical value, x_c, ($x < x_c$), the small particle will collide with the large particle and formed a closed trajectories. For $x > x_c$, there will be no collision. The value of x_c, however, is relatively small when compared with that for Region 1. Region 3 ($\Delta\rho_{cr2} < \Delta\rho_r < R_r^{-2}$ or $w_{cr} < w_r < 1$): for $x > x_c$, there is still no collision. For $x < x_c$, however, the small particle appears to be moving in a close loop near the downstream side of the large particle. The size of x_c is smaller than that for Region 2. Because of the cyclic motion, collision and separation will happen repeatedly. Although there is periodical contact between these two particles and some of the time there is no contact, these two particles cannot move together, and thus, it is not considered as one aggregate. Region 4 ($\Delta\rho_r > R_r^{-2}$ or $w_r > 1$): there is no chance of collision because the small particle would fall faster than the large particle. From the relative trajectory of two particles under different conditions, they concluded that the collision efficiency of these two settling particles depends on the ratio of their relative density and relative radius. However, this theoretical approach only considers the fluid-solid interactions, while the possible intermolecular forces are excluded.

When flocculation process involves small particles, the intermolecular forces should be included. Toward that direction, Davis (1984) contributed to the understanding of particle trajectories by including van der Waals force only, but he only found asymptotic solutions (although complemented by numerical computations) of the trajectories.

For particles with the same density and various size ratios, Jeffrey and Onishi (1984) developed an analytical solution to describe the interactions between fluid and solid particles. Their study, however, was also limited to large particles so that the intermolecular forces could be ignored. Based on Jeffrey and Onishi (1984)'s results, Han and Lawler (1991) added the intermolecular forces to extend the application for small hydrosol or aerosol systems. But their effort was still limited by the assumption of the same (or near the same) density for both particles.

Two decades after Wacholder and Sather's (1974) contribution, Stolzenbach and Elimelich (1994) conducted a laboratory experiment using a small solid glass sphere (diameter = 3 mm) and a large hollow plastic sphere (diameter = 17.4 mm) settling in glycerin to test the analytical solution given by Wacholder and Sather (1974). It is important to notice that the particles they selected are rather large. Although this is excellent for verifying the analytical solution, the intermolecular forces, which prevail among small particles, are still excluded. Nevertheless, their experimental results suggested that the analytical solution can be used as a ground truth to verify any numerical simulation of two-particle collision during differential settling when inter-molecular forces can be omitted.

Mazzolani et al. (1998) combined the influences of particle size ratio, submerged particle density ratio, and the action of van der Waals force, but included neither the electrostatic repulsion force nor the displacement force, to study the coagulation of spherical particles for differential settling in low Reynolds number and low Stokes number flows (i.e., with negligible fluid and particle inertia). Their predicted particle trajectories indicated that the collision efficiency decreases when the submerged particle density ratio increases. Similar results have been obtained by Leppinen (1999) and Chang and Hunag (2008) when the effects of van der Waals force and electrostatic repulsion force are included.

As an extension for other practical applications, Aziz et al. (2003) and Kim and Stolzenbach (2004) both studied the importance of permeability of large flocs' free falling in waters. Their numerical simulation results found that collision efficiency will be