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Numerical Investigation of the Agglomerating Behavior of Particles Governed by van der Waals forces

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ABSTRACT

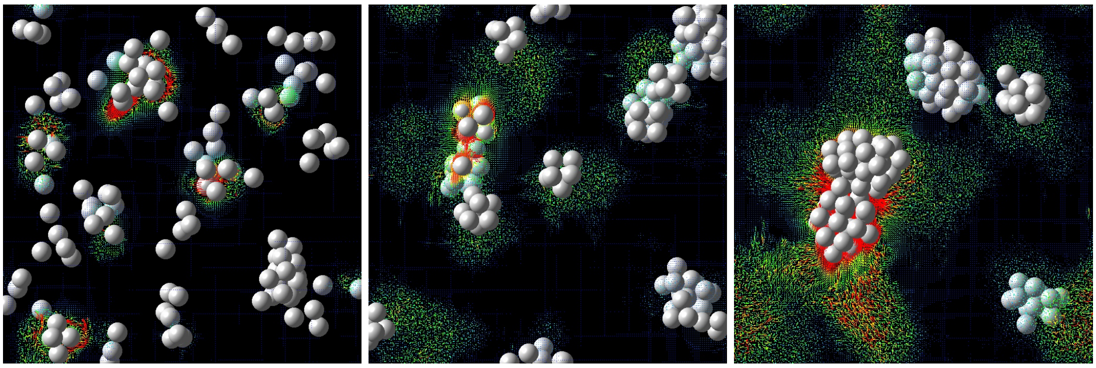
Flows involving particle agglomerates are often observed in environmental, industrial and biomechanical problems. The motion of particles becomes more complicated with decreasing the size of the particles, and the flows including these particles often exhibit various characteristics over a wide range of temporal and spatial scales. Therefore, the behavior of the system is difficult to predict, and numerical simulations, especially employing point-source-based models, for the motions of particles could be less accurate for analyzing the behaviors of the particles under the effect of non-sphericity and inter-particle and hydrodynamic forces.

The present authors developed a method to simulate particle-induced flows. We employ the treatment of interaction between the solid and fluid phases, which is used in the present study[1, 2]. Particle motions are solved individually by the equation of linear and angular momentums, and the fluid phase is solved by direct numerical simulation resolving from the boundary layer of the particle surface to the far wake. Interaction between the solid and fluid phases is treated by an immersed boundary method (IBM) proposed by Kajishima et al[1, 2]. The numerical technique has enabled investigation of the isolated effect of the dominant parameters for agglomerating and dispersing behaviors of the particles by simply switching on and off the parameters[3].

In the present study, we show some results obtained by the direct numerical simulation of 3-D flow induced by the motion of mono-sized particles involving inter-particle forces. For the inter-particle force, a van der Waals potential is used. This potential force models the attractive force to reach infinity as two particles approach to each other. Therefore, in the numerical implementation, the inter-particle force is turned off when the surface-to-surface distance of the two particles becomes smaller than the particle radius. This ad-hoc treatment, however, replicates the physical system very well as the agglomerating particles, in practice, experience some repulsive forces in addition to van der Waals forces. When

more than two particles come into contact, the contacting forces are calculated by a spring-dashpot model, known as a soft-particle model[4]. Figure 1 shows some snapshots of particle agglomeration and surrounding flow field. Initially, 125 particles are suspended in a static fluid in this example. Some particles gradually form nuclei of agglomerates (Figure 1(a)). Bigger agglomerates are observed as the primary particle structures attract each other(Figure 1(b)). A few big agglomerates coalesce with each other (Figure 1(c)). In this case, only van der Waals potential is applied as an interaction between particles, therefore agglomerates finally coalesce into a big one. The authors succeeded simulation of agglomerating particles of a total number of several thousands.

When the sizes of particles are in a submicron range, we should consider the effect caused by a high Knudsen number. The present fully-resolved simulation results suggest that the present approach, with an appropriate correction on the treatment of the fluid's boundary condition at the interface, should provide the basis for analyzing the flow field of a high Knudsen number.



(a) t^*=2.3 (b) t^*=6.5 (c) t^*=10.1

Figure 1: Sequential snapshots of agglomerating particles and surrounding flow fields (side views). The colored vectors show velocity vectors on a vertical cross section, and the color of the vectors represents the magnitude of velocity vectors.

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