Direct Numerical Simulation of the Dynamics of Colloidal Particles with Adsorptive Solute Transport

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Introduction

Additive solutes affect the dispersion stability, or interparticle forces in colloidal suspensions. In particular, soluble polymers are adsorbed onto the surface of colloidal particles to form thick adsorption layers, whose overlapping causes additional interparticle forces such as the attractive bridge force and the steric repulsive force. This phenomenon is utilized for stabilization of colloidal suspensions in various industrial fields; it is important to understand solute adsorption effects on the dynamics of colloidal particles.

The dynamics of colloidal particles is appropriately investigated by constructing a mesoscale model of the colloidal suspension system, in which the coupling motions of fluid and particles are considered. In such a model, the hydrodynamic interactions among colloidal particles mediated by the motion of the surrounding fluid can be exactly evaluated. To solve the governing equations in the mesoscale model, several direct numerical simulation approaches have been devised. In recent years, we have constructed an efficient direct numerical simulation scheme based on the immersed boundary method (IBM) [1, 2]. In the present study, we develop the mesoscale model and simulation scheme to be able to consider the solute transport and adsorption onto the surface of colloidal particles.

Model and simulation method

We model a colloidal suspension as a system in which spherical particles are dispersed in a Newtonian fluid. The host fluid contains a single solute species that can be adsorbed onto the surface of the particles. The solute adsorption is modeled by a square-well potential that represents a short-range attractive interaction between particle and solute. As governing

equations of the present model, the temporal evolutions of colloidal particles, solute, and host fluid are described by the Newton-Euler equations of motion, advection-diffusion equation, and Navier-Stokes equations, respectively; these equations are coupled each other. As for the solute transport, advection by fluid flow is considered, and boundary conditions are imposed on diffusion flux by solute impermeability and adsorptive property to the particles. As for the motions of fluid and particles, particle-solute interaction and osmotic pressure in the adsorption layer affect the fluid-particle momentum exchange.

The direct numerical simulation method to solve the governing equations is based on the IBM, in which boundary conditions of fluid flow are imposed by adding body forces on the particle domains. To indicate the particle domains, we introduce a phase function, which is equal to unity at the particle domain and zero at the fluid domain. The two regions are smoothly connected through thin interfacial regions with finite thickness to represent the spherical particle domain on the discrete computational grids. In the present development, we also introduce the phase function for the adsorption layers around particles; boundary conditions on diffusion flux are imposed by use of the phase functions for the particles and adsorption layers.

Simulation results

We give a simulation result of an interparticle force generated by the overlap of adsorption layers with equilibrium solute concentration distribution. Figure 1 shows the interparticle force as a function of the center-to-center distance between two particles L. We set the adsorption layer thickness and adsorption energy as $w/a = 0.5$ and $\varepsilon/RT = 0.5$, respectively, where a is the particle radius, T is the temperature, and R is the gas constant. As shown in Fig. 2, there are high solute concentration regions, or adsorption layers, in the vicinity of the particles. The overlapping of adsorption layers leads to increased solute concentration, where the particle-solute interaction is enhanced; therefore, an attractive force is generated between particles [Fig. 2(a)]. However, when two particles get closer, one particle faces to the adsorption layer of the other where it goes through high osmotic pressure due to high solute concentration; therefore, a repulsive force is generated between particles [Fig. 2(b)]. Consequently, there exists an equilibrium interparticle distance as $L/a \approx 2.35$, and particles are expected to assemble with some interparticle separation.
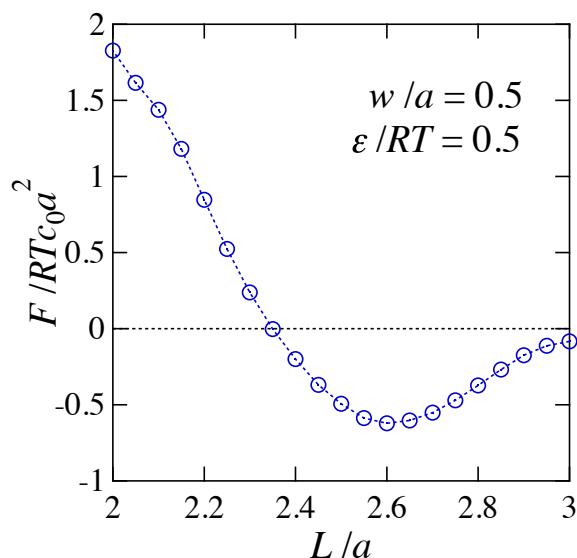
Fig. 1 Interparticle force caused by adsorption layer overlap vs. the distance between particle centers. A positive value ($F > 0$) means that the force is repulsive. The force is scaled by the osmotic pressure of dilute solution $c_0 RT$, where c_0 is the solute concentration in bulk.
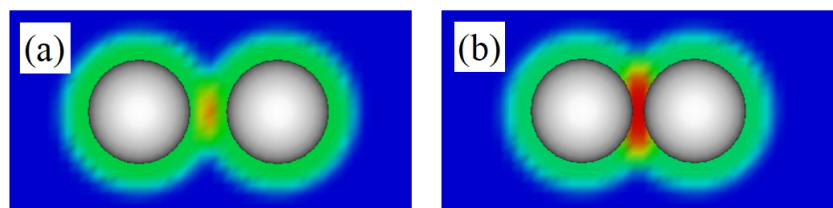

Fig. 2 Adsorption layer overlap. The increase in the solute concentration is expressed by the color change: blue → green → red.

Conclusion

We developed a simulation model to investigate the dynamics of colloidal particles with adsorptive solute transport. In this model, solute adsorption generates an additional interparticle force that changes non-linearly with depending on the interparticle distance. The present model will be applicable to the investigation in a drying process where fluid flow and inhomogeneous solute concentration distribution exist.

References

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[2] SNAP, a simulator for a basic process design, *http://nanotech.t.u-tokyo.ac.jp*