3차원 입자계 수치모사의 CONNFFESSIT-like 접근법

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A new CONNFFESSIT-like approach for 3D simulation of particulate systems

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Introduction

Brownian dynamics simulation has been generally used for the particulate system. But, if we consider many-body hydrodynamics in suspension system, it is very difficult to solve the flow field. Also, the simultaneous simulation of colloidal particles and liquid molecules is nearly impossible because the characteristic times of the colloidal particle motion and liquid molecule motion is significantly different. Therefore, this Brownian dynamics simulation is not practical for that kind of complex flow.

In the last decade, new approaches for modeling "meso-scale particle simulation" have appeared like Lattice-Boltzmann, Dissipative Particle Dynamics, and Fluid particle dynamics. Lattice Boltzmann method and dissipative particle dynamics use the virtual fluid particles instead of liquid molecules. The virtual fluid particle means a collection of liquid molecules. Although these methods can describe hydrodynamics between colloidal particles and liquid in the LBM and DPD, to simulate colloidal particles of a certain number, we need much more fluid particles because colloidal particles should be surrounded by enough fluid particles. Therefore, massive calculation of particle interaction is needed, and with the same reason, possible vol. fraction of suspension is limited. On the other hand, fluid particle dynamics uses the viscous underformable fluid particle as a colloidal particle. And interparticle interaction directly affects macroscopic the flow field. It circumvents the computational problem of LBM, DPD by using macroscopic simulation for flow field, But it also has a computational limit because the very fine mesh is needed even in the inside of all colloidal particles.

In this study, we develop a new platform for the mesoscale simulation of the particulate system which consider the interaction between colloidal particles and liquid molecules keeping macroscopic approach for the flow field. As a preliminary work, simple shear flow simulation is performed. Then, we compare the simulation results with that of Brownian dynamics simulation and discussed the hydrodynamic effects on particle microstructure.

Theory and governing equations

We introduce a new mesoscale simulation tool for spherical particle suspensions based on CONNFFESSIT (Calculation Of Non-Newtonian Flows: Finite Elements and Stochastic Simulation Technique)-like algorithm which is a stochastic simulation as an alternative to the conventional macroscopic simulation. In this approach, in order to take the complex hydrodynamics of flowing particles into account, Brownian dynamics (BD) simulation technique has been combined with finite element method (FEM). That is, the flow field obtained from FEM is used to BD simulation and the particle stress contribution obtained from BD simulation is used to solve the flow field by FEM.

The governing equations consist of for the particle simulation and the conservation equations, that is, Navier-Stokes equation and continuity equation.

In particle simulation, the motion of particle is governed by friction force, potential force, and Brownian force.

$$m\frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{F}_i^{fric} + \boldsymbol{F}_i^{pot} + \boldsymbol{F}_i^{Br} \tag{1}$$

As an interparticle force, Lennard-Jones force was used.

$$U = A\varepsilon\left[\left(\frac{d}{r}\right)^{12} - \left(\frac{d}{r}\right)^{6}\right], \quad F^{Pot} = -\frac{dU}{dr} \tag{2}$$

If we use Stokes drag force as a friction force and neglect inertia, we can get a following differential equation.

$$d\boldsymbol{r}_i = \left[\boldsymbol{v}_i^{\infty} + \frac{1}{\zeta}\boldsymbol{F}_i^{Pot}\right]dt + \sqrt{\frac{2k_BT}{\zeta}}dW, \quad \langle dW\rangle = 0, \langle dWdW'\rangle = \delta(t-t')Idt, \tag{3}$$

where, $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$ are the position and velocity vectors of i_{th} particle, respectively. $\boldsymbol{v}_i^{\infty}$ denotes the imposed flow field at i_{th} particle position and ζ is drag coefficient.

In conservation equations of momentum and mass, the extra stress of the colloidal particles is defined by averaging of $\boldsymbol{rF}$ and used in Navier-Stokes equation.

$$-\nabla p + \nabla\cdot\boldsymbol{\tau}_p + \eta\nabla^2\boldsymbol{v}^{\infty} = 0, \quad \boldsymbol{\tau}_p = -\frac{1}{V}\sum_{i=1}^{N}\boldsymbol{r}_i\boldsymbol{F}_i^{Pot}$$
$$\nabla\cdot\boldsymbol{v}^{\infty} = 0 \tag{4}$$

For the convenience of calculation, we take dimensionless forms using the following characteristic length, time, force scale.

$$l_{scale} = d = 2a; \quad 4d(=8a)$$
$$t_{scale} = \frac{l_{scale}^2}{D} = \frac{l_{scale}^2 \zeta}{kT}$$
$$F_{scale} = \frac{kT}{l_{scale}} \qquad (5)$$

where d is the particle diameter, a is the particle radius, and D is diffusion coefficient, respectively.
Then, we can get the final dimensionless equations.

$$dr_i = \left[v_i^{\infty} + F_i^{Pot} \right] dt + \sqrt{2} dW$$
$$-\nabla p + \nabla \cdot \tau_p + \frac{1}{6\pi a} \nabla^2 v^{\infty} = 0, \quad \tau_p = -\frac{1}{V} \sum_{i=1}^{N} r_i F_i^{Pot}$$
$$\nabla \cdot v^{\infty} = 0 \qquad (6)$$

If we assume that the particles are sufficiently large, we can neglect this Brownian motion term. The flow field v^{∞} can be solved by finite element method. Then it is used in particle simulation to calculate the particle positions and the interparticle forces which are used in solving conservation equation again.

Results and discussion

Through CONNFFESSIT-like approach, simple shear flow simulation was performed as a preliminary work and we compared the simulation results with those of BD simulation. In hexahedron simulation domain, suspension including 165,888 particles with 0.113 vol. fraction was simulated. The mesh of finite element method has 490 elements.
As a result, viscosity level is lowered by CONNFFESSIT-like approach as in Fig. 1.

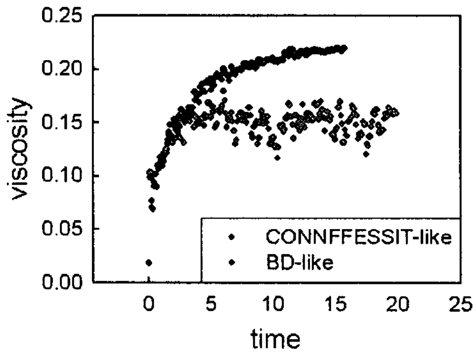

Fig. 1. The viscosity levels by CONNFFESSIT-like approach and BD simulation.

Then, we analyzed the cluster size and its distribution to see the microstructural difference leading to the viscosity difference. We could confirm that more diffusive morphology is constructed in CONNFFESSIT-like approach than in BD simulation.
Also, we performed the cluster analysis by fractal dimension. In fractal structure, cluster weight is a power law function of the radius of gyration.

$$M \propto R_g^{D_f} \qquad (7)$$

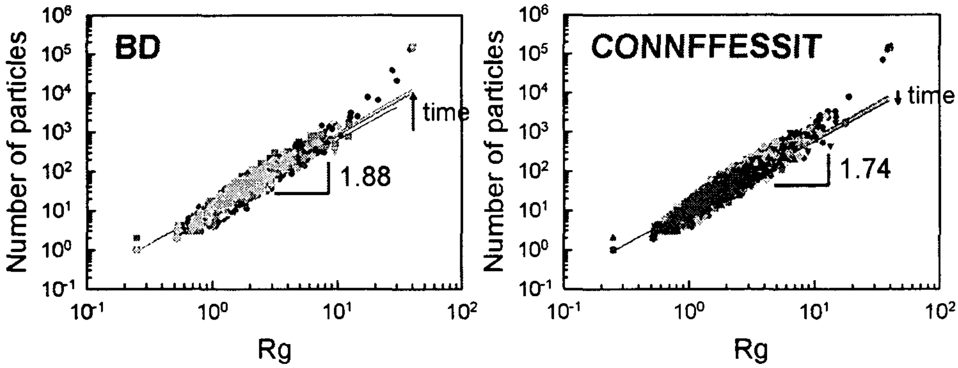

Fig. 2. The fractal dimensions for the simulation results of CONNFFESSIT-like approach and BD.

In CONNFFESSIT approach, lower fractal dimension was obtained than in BD simulation as time goes by. That is to say, smaller and more distributed cluster morphology is constructed in CONNFFESSIT approach, and this configurational change induces lower stress level. It is caused by the hydrodynamic effect which changes the local velocity field leading to more coarse particle configuration even in simple shear flow.
Through this combination of particle simulation and flow field as CONNFFESSIT-like approach, we can apply and interpret complex suspension behavior keeping their interactions.

References

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