

Computer simulation of distributions and structure formations of magnetic spherocylinder particles and nonmagnetic sphere particles in MAGIC fluid under steady magnetic field

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Distribution of magnetic spherocylinder particles and nonmagnetic sphere particles in MAGIC (MAGnetic Intelligent Compound) fluid under steady magnetic field is examined using the particle method. In order to arrange nonmagnetic abrasive particles to the applied magnetic field direction, using magnetic spherocylinder particles is effective. In particular, particle distribution on the plane perpendicular to the field direction is more uniform compared to the case using magnetic sphere particles.

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1. Introduction

Magnetic particles of micron size form clusters in the presence of an external magnetic field [1, 2]. MAGIC (MAGnetic Intelligent Compound) is one of applications using this phenomena. MAGIC is a solidified magnetorheological fluid containing both magnetic particles and nonmagnetic abrasive particles of micron size [3]. Distribution of nonmagnetic abrasive particles can be controlled by changing physical conditions of solidifying process. Thus, it is important to know how these particles are arranged in applied magnetic field, because distribution of nonmagnetic abrasive particles dominates MAGIC polishing. The authors have reported the distribution and structure formation of sphere particles in MAGIC fluid [4, 5]. We have shown that cluster formation of sphere particles in MAGIC fluids under applied steady magnetic field is useful to arrange abrasive particles to the direction of applied magnetic field.

In this paper, we investigate distribution and microstructure formation of magnetic spherocylinder particles and spherical abrasive particles in MAGIC fluids under steady uniform magnetic field. This work is based on the idea that using the magnetic particles with rod-like shape is more suitable for arranging the abrasive particles to the direction of applied magnetic field. The distribution and structure formation of particles are analyzed statistically.

2. Simulation method

A three-dimensional system to be simulated is based on a magnetic pole model for magnetic particles and the

simple Stokesian model [1]. We use a hard particle picture without full hydrodynamic effects through the medium such as many-body hydrodynamic interactions, lubrication force and buoyancy. The rod-like magnetic particles are modelled as spherocylinders with diameter d and length l as shown in Fig. 1, while nonmagnetic abrasive particles are considered as spheres with diameter d . The aspect ratio of the spherocylinder particles is $l/d = 1$ (spherical particle), 2 and 3 in our simulations. These particles are arranged randomly in a box with $10d \times 10d \times 20d$ ($10d \times 10d \times 10d$ in case of the aspect ratio of 1) at the initial state. The number of particles is, for example, 300 magnetic particles and 600 nonmagnetic particles in case of the aspect ratio of 2 and the volume fraction ratio of 0.5. An external uniform steady magnetic field is applied to the z -direction and a periodic boundary condition is imposed in all directions. The motion of the i th particle having mass m_i at time t and position \mathbf{r}_i is described by using the following equations:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i - \frac{k_B T}{D_i^t} \frac{d\mathbf{r}_i}{dt} + \mathbf{R}_i, \quad (1)$$

$$I_i \frac{d\boldsymbol{\Omega}_i}{dt} = \mathbf{T}_i - \frac{k_B T}{D_i^r} \boldsymbol{\Omega}_i + \mathbf{N}_i, \quad (2)$$

where k_B is the Boltzmann constant, T is the absolute temperature, D_i^t and D_i^r are the diffusion coefficients for translational and rotational motion [6], I_i is the inertia

moment of the particle, $\boldsymbol{\Omega}_i$ is the angular velocity, \mathbf{R}_i and \mathbf{N}_i are Brownian force and torque, respectively. The force \mathbf{F}_i is the total force acting on the particle and it includes magnetic pole interactions and short-range repulsive forces based on the DLVO theory. \mathbf{T}_i is the total torque acting on the particle. In our simulations, Brownian force and torque are ignored. The total force is given by

$$\mathbf{F}_i = \sum_{j(\neq i)} \mathbf{F}_{ij}^M + \sum_{j(\neq i)} \mathbf{F}_{ij}^{rep} + \sum_k \mathbf{F}_{ik}^{rep}, \quad (3)$$

where subscript j indicates the magnetic particles and subscript k indicates the nonmagnetic particles. The magnetic pole interaction force \mathbf{F}_{ij}^M and the repulsive force \mathbf{F}_{ij}^{rep} are expressed, respectively, by

$$\mathbf{F}_{ij}^M = \frac{\xi_i \xi_j}{4\pi\mu_0} \left(\frac{\mathbf{r}_i^+ - \mathbf{r}_j^+}{|\mathbf{r}_i^+ - \mathbf{r}_j^+|^3} + \frac{\mathbf{r}_i^- - \mathbf{r}_j^-}{|\mathbf{r}_i^- - \mathbf{r}_j^-|^3} - \frac{\mathbf{r}_i^+ - \mathbf{r}_j^-}{|\mathbf{r}_i^+ - \mathbf{r}_j^-|^3} - \frac{\mathbf{r}_i^- - \mathbf{r}_j^+}{|\mathbf{r}_i^- - \mathbf{r}_j^+|^3} \right), \quad (4)$$

$$\mathbf{F}_{ij}^{rep} = \frac{3\xi_S^2}{4\pi\mu_0 d^4} \exp(-\kappa S) \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|}, \quad (5)$$

where μ_0 is the magnetic permeability in vacuum, ξ_S is the saturated magnetization of the magnetic particles, S is the distance between the surfaces of two particles, κ is corresponding to the Debye-Hückel parameter ($\kappa = 15$ in our simulations), $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, ξ_i is the magnetic moment given by

$$\xi_i = \frac{d^3 \pi}{2} \frac{\mu - \mu_0}{\mu + 2\mu_0} \mathbf{B}, \quad (6)$$

in a weak magnetic field of magnetic flux density \mathbf{B} . The total torque is given by

$$\mathbf{T}_i = \sum_{j(\neq i)} \mathbf{T}_{ij}^M + \mathbf{T}_i^{field}, \quad (7)$$

where \mathbf{T}_{ij}^M is the torque due to the magnetic pole interaction force and \mathbf{T}_i^{field} is the torque due to the interaction between applied magnetic field and magnetic moment of the particles: $\mathbf{T}_i^{field} = \xi_i \times \mathbf{H}$, where \mathbf{H} is the magnetic field intensity vector.

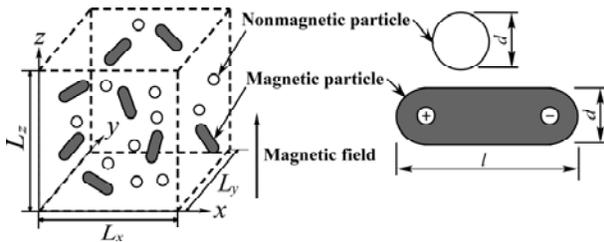


Fig. 1. Analytical model of MAGIC fluid.

We introduce scale unit of some physical quantities: the unit of length as d , force as $3\xi^2 / 4\pi\mu_0 d^4$, time as $t_0 = m / 3\pi\eta d$, where m is the mass of the spherical magnetic particle, and angular velocity as $3\pi\eta d / m$. The equations of motion (1) and (2) can be rewritten as the following dimensionless forms:

$$m_i^* \frac{d\mathbf{r}_i^*}{dt^*} = D_i^* A \mathbf{F}_i^*, \quad \boldsymbol{\Omega}_i^* = 3D_i^* A \mathbf{T}_i^*, \quad (8, 9)$$

where the parameters A is defined by

$$A = \frac{\rho d^2}{288\mu_0 \eta^2} \left(\frac{\mu - \mu_0}{\mu + 2\mu_0} B \right)^2. \quad (10)$$

The parameter A is constant of 10^4 in our simulations. The translational and rotational diffusion coefficients are depend on the particle shape. The simple Euler method with a time step $10^{-9} t_0$ is used to integrate the above equations (8) and (9).

3. Results and discussions

The particle method simulation is carried out to investigate microstructure formation of interacting magnetic spherocylinder particles and nonmagnetic sphere particles. Simulations are conducted on three different aspect ratios of the spherocylinder particles, 1, 2 and 3, and four different ratios of volume fraction of magnetic particles to the total volume fraction of particles, 0.25, 0.50, 0.75 and 1.00. Total volume fraction of particles is 0.32.

Figs. 2, 3 and 4 are the snapshots of bird's eye views of distribution of particles. Fig. 5 is the snapshots of top views of distribution of particles. The final steady states are after 10^5 steps. When the aspect ratio is 1, magnetic particles rapidly form isolated chain clusters in case of low fraction of magnetic particles, while magnetic particles form wall-like structure in case of higher volume fraction. However, we cannot see any organized structures of magnetic spherocylinder particles when the aspect ratio is 2 or 3.

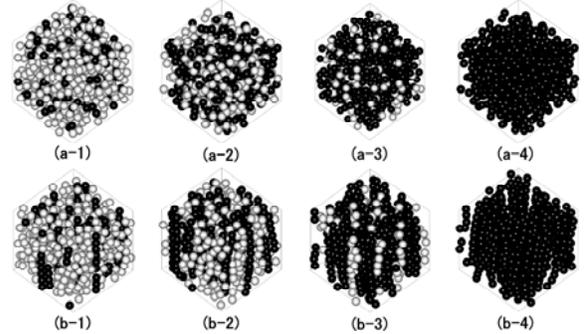


Fig. 2. Snapshots of distribution of particles. The aspect ratio of the spherocylinder particles is 1. (a) The initial state and (b) steady state. The ratio of volume fraction of magnetic particles to that of all particles $\phi_{\text{mag}} / \phi_{\text{all}}$ is (1) 0.25, (2) 0.50, (3) 0.75 and (4) 1.00, respectively. The black particles are magnetic particles.

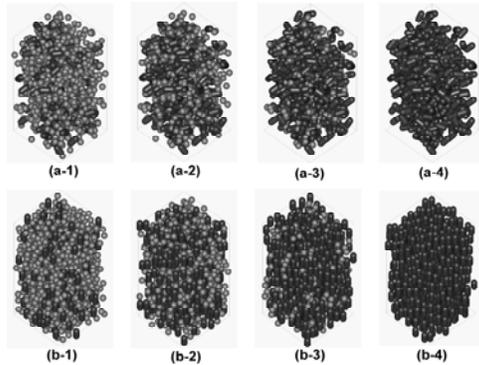


Fig. 3. Snapshots of distribution of particles. The aspect ratio of the spherocylinder particles is 2. (a) The initial state and (b) steady state. The ratio of volume fraction of magnetic particles to that of all particles $\phi_{\text{mag}} / \phi_{\text{all}}$ is (1) 0.25, (2) 0.50, (3) 0.75 and (4) 1.00, respectively. The black particles are magnetic particles.

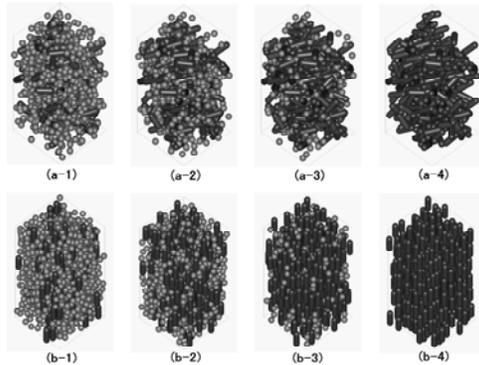


Fig. 4. Snapshots of distribution of particles. The aspect ratio of the spherocylinder particles is 3. (a) The initial state and (b) steady state. The ratio of volume fraction of magnetic particles to that of all particles $\phi_{\text{mag}} / \phi_{\text{all}}$ is (1) 0.25, (2) 0.50, (3) 0.75 and (4) 1.00, respectively. The black particles are magnetic particles.

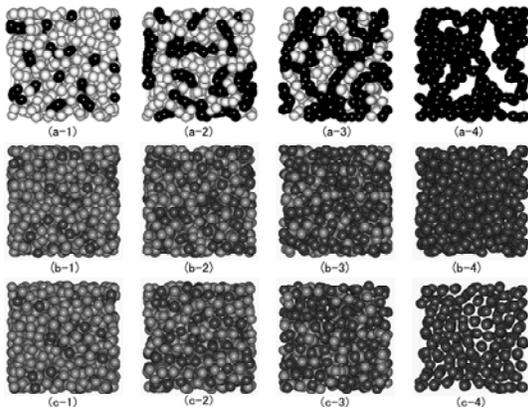


Fig. 5. Snapshots of the top view of particle distribution. The aspect ratio is (a) 1, (b) 2 and (c) 3. The ratio of volume fraction of magnetic particles to that of all particles $\phi_{\text{mag}} / \phi_{\text{all}}$ is (1) 0.25, (2) 0.50, (3) 0.75 and (4) 1.00, respectively. The black particles are magnetic particles.

In order to analyze the microstructure of particles statistically, we defined some coefficients. We define the modified contact coefficient C_v which is the ratio of the number of contacts between particles to the field direction against the number of contacts when all particles form chain clusters (e.g. if all particles form chain clusters, i.e., all particles are members of chain clusters, $C_v = 1$). The number of contacts is counted when the surface distance between the target particle and the neighbour particle is within the cut-off distance r_c . Fig. 6 demonstrates the contact coefficients for magnetic particles ($r_c = 0.1d$) and nonmagnetic particles ($r_c = 0.5d$), respectively. As we can see in Fig. 6, both magnetic particles and nonmagnetic particles form chain-like structures under applied magnetic field, even when any organized structure cannot see in case of the aspect ratio of 2 and 3. From Fig. 6, even when the volume fraction of magnetic particles is small, nonmagnetic particles are arranged along the field direction.

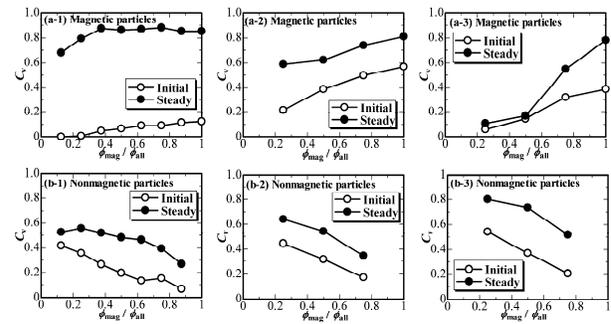


Fig. 6. Contact coefficients of (1) magnetic particles and (2) nonmagnetic particles. The aspect ratio of the magnetic particles is (a) 1, (b) 2 and (c) 3.

In order to examine uniformity of distribution of particles, Christiansen's uniformity coefficient [7] is defined by $CU_L = (1 - D_L / M_L) \times 100$,

$$\text{where } D_L = \sum_{i=1}^{N_L} (d_{i,L} - M_L) / N_L \text{ and } M_L = \sum_{i=1}^{N_L} d_{i,L} / N_L,$$

N_L is the number of particles existing on the L th plane and $d_{i,L}$ is the mean distance between the particle and the surrounding particles on the L th plane. Fig. 7 shows the averaged Christiansen's uniformity coefficient for magnetic particles and nonmagnetic particles. From Fig. 7, the averaged Christiansen's uniformity coefficients under applied magnetic field is almost the same as those of the initial state. The uniformity is kept even after particles move by applying magnetic field.

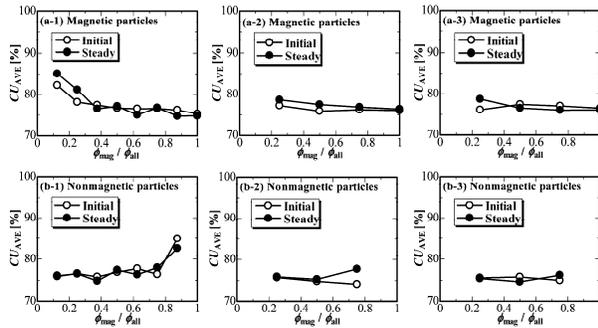


Fig. 7. Christiansen's uniformity coefficients for (1) magnetic particles and (2) nonmagnetic particles. The aspect ratio of the magnetic particles is (a) 1, (b) 2, and (c) 3, respectively.

The standard deviation of Christiansen's uniformity coefficient is defined by $\Delta CU = \sqrt{\sum_{l=1}^{N_L} (CU_{AVE} - CU_L)^2}$.

If the standard deviation is small, almost the same surface appears at any time when we use it as a polishing pad. Fig. 8 illustrates the standard deviation of Christiansen's uniformity coefficient. It is evident from Fig. 8 that deviation is more reduced in case of the aspect ratios of 2 and 3 compared with the case of aspect ratio of 1 (magnetic sphere particles). This means that the magnetic spherocylinder particles are effective to form the MAGIC abrasive pad whose structure to the field direction is uniform.

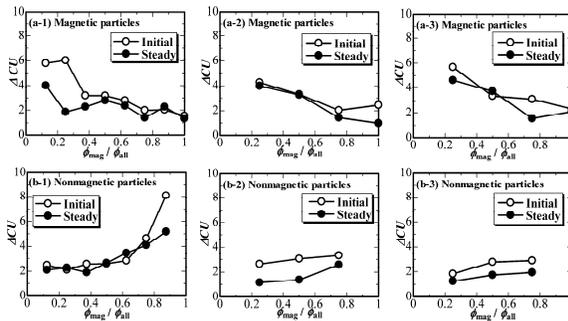


Fig. 8. Standard deviation of Christiansen's uniformity coefficients for (1) magnetic particles and (2) nonmagnetic particles. The aspect ratio of the magnetic particles is (a) 1, (b) 2, and (c) 3, respectively.

4. Conclusions

Performing the particle method analysis, we have simulated various ordering processes and microstructure formations in MAGIC fluids. It is shown that the nonmagnetic particles are arranged to the field direction due to the structure formation of magnetic spherocylinder particles in applied magnetic field. We found that the magnetic spherocylinder particles are very useful to produce the MAGIC polishing pad with better uniformity to the field direction even when the volume fraction of magnetic particles is small.

Acknowledgments

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