Numerical Analysis of Microstructure Formation of Magnetic Particles and Nonmagnetic Particles in MR Fluids

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Abstract. Microstructure formation of magnetic particles and nonmagnetic particles in MR fluids is investigated using the particle method simulation. Nonmagnetic sphere particles are rearranged in the field direction due to the chain-like cluster formation of magnetic particles. In the contrast, the nonmagnetic spherocylinder particles are not sufficiently rearranged in the field direction by using the cluster formation of sphere magnetic particles.

1. Introduction
Magentic particles of micronsize form clusters in MR fluids in the presence of magnetic field [1]. Microstructure formation of suspended particles in MR fluids is very interesting problem in physics, chemistry, and engineering. Nonmagnetic particles in MR fluids are also rearranged by applying magnetic field due to the cluster formation of magnetic particles. Magnetic intelligent compound (MAGIC) is one of applications using this phenomenon [2]. In the previous papers [3,4], we have reported that the effects of the volume fraction of particles on the distribution of suspended particles in MR fluids containing nonmagnetic particles. In this paper, we report the microstructure formation of both magnetic particles and nonmagnetic particles in MR fluids. We investigate the influence of both size and shape of particles (both of magnetic particles and of nonmagnetic particles) in the presence of uniform steady magnetic field.

2. Numerical method
A three-dimensional system to be simulated is based on a magnetic pole model for magnetic particles and the simple Stokesian model. We use a hard particle picture without full hydrodynamic effects through the medium such as many-body hydrodynamic interactions, lubrication force and buoyancy. In our simulations, particles are sphere or spherocylinder particles. Figure 1 shows the analytical model of our simulations. When the magnetic particles are sphere, we use the dipole model, while the poles model is used in case of the spherocylinder magnetic particles. All particles are arranged randomly in the initial state. Uniform steady magnetic field is applied in the z-direction and 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.

\[
m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i - k_B T \frac{d \mathbf{r}_i}{dt} + \mathbf{R}_i,
\]

\[
I_i \frac{d\Omega_i}{dt} = \mathbf{T}_i - k_B T \frac{d\Omega_i}{dt} + \mathbf{N}_i,
\]

where \(k_B\) is the Boltzmann constant, \(T\) is the absolute temperature, \(D_t^i\) and \(D_r^i\) are the diffusion coefficients for translational motion and rotational motion \([5]\), \(I_i\) is the moment of inertia, \(\mathbf{R}_i\) and \(\mathbf{N}_i\) are Brownian force and torque which are independently calculated by using Box-Müller method, and \(\Omega_i\) is the angular velocity. The total force \(\mathbf{F}_i\) and the total torque \(\mathbf{T}_i\) for the magnetic particles are given by the following equations:

\[
\mathbf{F}_i = \sum_{j(\neq i)} \mathbf{F}^M_{ij} + \sum_k \mathbf{F}^{rep}_{ik}, \quad \mathbf{T}_i = \sum_{j(\neq i)} \mathbf{T}^M_{ij} + \mathbf{T}^{field}_i
\]

while the total force and the total torque for the nonmagnetic particles are given by the following equations:

\[
\mathbf{F}_k = \sum_i \mathbf{F}^{rep}_{ik} + \sum_k \mathbf{F}^{rep}_{kl}, \quad \mathbf{T}_i = 0
\]

where subscripts \(i\) and \(j\) are the numbers of magnetic particles, subscripts \(k\) and \(l\) are the numbers of nonmagnetic particles. The magnetic force \(\mathbf{F}^M_{ij}\) is the dipole-dipole interaction in case of spherical magnetic particles, while \(\mathbf{F}^M_{ij}\) is the magnetic pole interaction force in case of the spherocylinder magnetic particles. The short-range repulsive force \(\mathbf{F}^{rep}_{ij}\) is based on the DLVO theory. The torque \(\mathbf{T}^M_{ij}\) is the magnetic torque due to the dipole interaction and \(\mathbf{T}^{field}_i\) is the magnetic torque due to the interaction between the magnetic moment of the particle and applied magnetic field.

The simple Euler method with a time step \(10^{-8} t_0\) is used to integrate the above equations (1) and (2), where \(t_0 = m/3\pi\eta d\), \(d\) is the diameter of magnetic particles, \(\eta\) is the viscosity coefficient.

We simulate microstructure formation of interacting magnetic particles and nonmagnetic particles. Simulations are conducted on three different aspect ratios of the spherocylinder particles: \(l/d = 1\) (spherical particle), 2 and 3, and six different ratios of diameter of spherical nonmagnetic particles to that of spherical magnetic particles: 0.5, 0.8, 1.0, 1.2, 1.5 and 2.0. The volume fraction of magnetic particles is 0.16 and that of nonmagnetic particles is 0.16. We assume that the MR fluid is composed of manganese zinc ferrite particles (diameter: 3\(\mu\)m, density: \(2.5 \times 10^3 \text{kg/m}^3\), saturated magnetization: 0.223T) and myristic myristate (density: 8.3\(\times\)
Figure 2. Snapshots of bird’s eye views of distribution of suspended particles in the presence of magnetic field. The dark particles are magnetic particles and the light particles are nonmagnetic particles. The ratio of the diameter of nonmagnetic particles to that of magnetic particles is (a) 0.5, (b) 0.8, (c) 1.0, (d) 1.2, (e) 1.5 and (f) 2.0. The aspect ratio of the spherocylinder particles is (g,i) 2.0 and (h,j) 3.0, respectively.

10^2 kg/m^3, viscosity: 1.5 × 10^{-4} Pa · s, melting point: 40°C) and the nonmagnetic particles are made of silicon carbide (density: 3.2 × 10^3 kg/m^3). The applied magnetic field and the temperature are assumed to be constant, 70mT and 70°C, respectively. In our simulations, the dependence of temperature on the distribution of particles is neglected.

3. Results and discussion

Figure 2 shows the snapshots of distribution of suspended particles in MR fluids after 10^5 time steps. As we can see in figure 2, both spherical magnetic particles and spherical nonmagnetic particles form chain-like clusters in the presence of magnetic field, while any organized structures of nonmagnetic particles cannot be seen in cases of the spherocylinder particles.

In order to analyze the distribution of particles statistically, we define the modified contact coefficient \( C_v \) [1,4]. The contact coefficient is the ratio of the number of contacts between the target particle and the other particles in the field direction against the number of contacts when all particles form chain-like clusters (e.g. if all magnetic or nonmagnetic particles form chain-like clusters, i.e., all magnetic or nonmagnetic particles are members of chain clusters, thus \( C_v = 1 \)). The number of contacts is counted when the surface distance between the target particle and the neighbour particle is within the cut-off distance \( r_c \). In case of the spherocylinder particles, the distance between the magnetic poles is less than \( d + r_c \) and the axis of the particle is inclined within 30° to the field direction, we count as contact in the field direction. In each cases shown in figure 2, \( C_v \) becomes almost stable after 10^5 steps.

Figure 3 illustrates the contact coefficients of spherical magnetic particles (\( r_c = 0.1d \)) and spherical nonmagnetic particles (\( r_c = 0.5d \)), respectively. Figure 4 demonstrates the contact coefficients of spherocylinder particles and spherical particles. From figures 3(1) and 4(1), we have found that magnetic particles are rearranged in the field direction and form chain-like clusters in almost all cases, because the differences between the initial \( C_v \) and the final \( C_v \) are
large. When all particles are sphere, from figure 3(2), nonmagnetic particles are also rearranged in the field direction. The increase of $C_v$ is the largest when the ratio of diameter is 0.8. Thus, slightly small nonmagnetic particles are suitable in order to form chain-like clusters of nonmagnetic particles in MR fluids. From figure 4(2), using spherocylinder magnetic particles is effective for rearranging spherical nonmagnetic particles in the field direction, while cluster formation of spherical magnetic particles cannot rearrange spherocylinder nonmagnetic particles in the field direction.

4. Concluding remarks
Performing the simple particle method analysis, we have simulated various ordering processes and microstructure formation of both magnetic and nonmagnetic particles in MR fluids. When spherical nonmagnetic particles are slightly small comparing with spherical nonmagnetic particles, more nonmagnetic particles are rearranged in the field direction. Using spherocylinder magnetic particles is effective to arrange spherical nonmagnetic particles in the field direction. In the contrast, cluster formation of spherical magnetic particles is not useful to rearrange

Figure 3. The modified contact coefficients. The ratio of diameter of nonmagnetic particles to that of magnetic particles is (a) 0.5, (b) 0.8, (c) 1.0, (d) 1.2, (e) 1.5 and (f) 2.0. The particles are (1) magnetic particles and (2) nonmagnetic particles. The open circles: initial state, and the closed circles: final state, respectively.

Figure 4. The modified contact coefficients. The aspect ratio of the spherocylinder particles is (a,c) 2.0 and (b,d) 3.0, respectively. The spherocylinder particles are (a,b) magnetic particles and (c,d) nonmagnetic particles. The open circles: initial state, and the closed circles: final state.
spherocylindrical nonmagnetic particles in the field direction.

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