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International Journal of Heat and Mass Transfer 48 (2005) 2443–2451
International Journal of HEAT and MASS TRANSFER
www.elsevier.com/locate/ijhmt

Mesoscale simulation of ferrofluid structure

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Received 20 August 2004; received in revised form 13 December 2004
Available online 29 March 2005

Abstract

By means of the lattice-Boltzmann (LB) method, the mesoscaled structure of ferrofluids consisting of magnetic nanoparticles and a carrier fluid as well as some surfactant is investigated. The ferrofluid is a complicated system and its morphology is affected by a number of internal and external forces including gravitational force, Brownian force, van der Waals attraction potential, and dipole–dipole interaction potential. All these factors are included in the lattice-Boltzmann model. The distribution of suspended magnetic nanoparticles and morphology of the ferrofluid are simulated in both cases of the absence and the presence of an external magnetic field. The effects of the dipole–dipole interaction energy and the thermal energy on the aggregation structures of the magnetic nanoparticles are discussed.

1. Introduction

Ferrofluids are composed of magnetic nanoparticles (3–15 nm) and carrier fluid. Such ultrafine particles may be coated by a suitable surfactant (activator or dispersant) to keep a stable suspension state and they can be treated as particles of single magnetic domain. Ferrofluids exert some unique performances under the influence of external magnetic fields, i.e. an applied magnetic field can be used to control physical and flowing properties of the ferrofluid. Ferrofluids behave as a smart or functional fluid and has been finding more and more applications in a variety of fields such as electronic packing, mechanical engineering, aerospace, bioengineering, and thermal engineering [1–4]. The distribution structure of the suspended nanoparticles remarkably affects the transport properties and heat transfer characteristic of the ferrofluid. With respect to the effect of an external magnetic field, such properties of the ferrofluid will be strongly anisotropic, which means that by means of an external magnetic field one can make flow and energy transport processes of the ferrofluid controllable.

Since the ferrofluid is a complicated ferromagnetic colloidal system, the suspended magnetic nanoparticles experience actions from a number of forces such as gravitational force, Brownian force, Stokes drag force, van der Waals attraction potential, and dipole–dipole interaction potential in the presence of an external magnetic field. All these acting forces and potentials dominate behavior and structure of the ferrofluid. To get insights into the morphology and performance of the ferrofluid, it is necessary to investigate its microstructure and the relevant affecting factors. The main method of investigating the microstructure of the ferrofluid is Brownian dynamics and molecular dynamics simulation [5,6]. These publications simulated the cluster aggregation of the particles and the structure of the ferrofluid by focusing attention on each particle and considering some forces (or potentials) acting on the particle. Obviously,

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doi:10.1016/j.ijheatmasstransfer.2004.12.039

Nomenclature

a	particle radius, m	N/V	number density of the particles
d_p	particle diameter, m	T	absolute temperature, K
k_B	Boltzmann constant, J/K	ω	Lorentz number, $\omega = \frac{1}{3}$
m	magnetic dipole moment of single particle, A m^2	μ_0	vacuum permeability, $\mu_0 = 4\pi \times 10^{-7}$ H/m
		μ	fluid viscosity, Pa s
M_d	bulk magnetization of the material, A/m	η	relaxation time

such a method is time consuming and is limited by a finite number of the suspended particles. The lattice-Boltzmann method originating from the Boltzmann equation became popular over the past few years [7]. It bridges the gap between the microscopic world and the macroscopic phenomenology and provides a possible approach for simulating flow and energy transport processes of a flow system at the mesoscaled level without particle limitation. As regards the multiscaled simulation algorithm for some system, the lattice-Boltzmann method is an intermediate between the molecular dynamics simulation for each microparticle and the Navier–Stokes equations for macroscaled simulation. It simulates fluid motion and energy transport by following the evolution of a prescribed Boltzmann equation instead of solving the Navier–Stokes equations. One of the important advantages of this method is that microscopic physical interactions among the fluid particles can be conveniently incorporated into the model. This method has been found recent successes in a lot of fluid dynamic problems, including flow in porous media [8], thermal two-phase flow [9] and diffusion in multicomponent fluids [10]. Sofonea and Frueh [11] proposed a lattice-Boltzmann model to investigate the competition relation between surface tension and dipolar interaction in magnetic fluids. By taking into account the effects of several forces and potentials acting on the suspended nanoparticles, this method has recently been introduced to simulate nanoparticle behavior in nanofluids [12].

From the point of microscopic view, there exist a number of forces and potentials acting on ferrofluids, for example, gravitational force, Brownian force, van der Waals attraction potential, magnetic field gradients, and dipole–dipole interaction potential. Some of them may bring magnetic nanoparticles together and form clusters, but the others may make nanoparticles move apart. It is these internal and external forces that affect and control the morphology of the ferrofluid and make the fluid have some unique features. In this paper, we apply the lattice-Boltzmann method to simulate the mesoscaled morphology of the ferrofluid by accounting for the effects of the acting forces and potentials on the ferrofluid structure, especially the effects of the magnetic dipole–dipole interaction energy and the kinetic energy. The paper is organized in the following way. In Section 2, some features and magnetization property of the ferrofluid are analyzed. The LB model for a multiple-component system is briefly introduced in Section 3. Section 4 is contributed to description of the interparticle potentials, Stokes drag force, Brownian force, and gravitational force are. Finally, some simulation results of a ferrofluid system with homogeneous ferromagnetic nanoparticles under the influence of all these forces are presented.

2. Magnetic features and magnetization property

The ferromagnetic nanoparticles suspended in the liquid carrier can generally be considered as a single magnetic domain because of their ultrafine sizes. The macroscopic features of the ferrofluid depend not only upon the properties of single suspended particles but also on the interactions among these particles. In the presence of an external magnetic field, the ferrofluid will be magnetized in the direction of the field and may easily approach saturation magnetization. Once the external field is removed, the ferrofluid magnetization will immediately vanish with a randomly oriented domain and show no macroscaled magnetism. It is for this reason that the ferrofluid is generally considered as being superparamagnetic. Such magnetization of the ferrofluid is related with the arrangement structure of the suspended magnetic nanoparticles. The external field forces attract the magnetic nanoparticles in a regular alignment, but the Brownian force always puts the nanoparticles in random motion and tries to keep them in an irregular structure. The external field will align the magnetic moment of the suspended particles along the field and lead to solid particle-carrier liquid separation. Among all the forces acting on the ferrofluid, the dipole–dipole interaction potential and the Brownian force are the two most important external factors of affecting the microstructure and magnetization process of the ferrofluid. In the case when an external magnetic field exists, the two main parameters of describing the features and performances of the ferrofluid are the volume fraction ϕ of the suspended magnetic nanoparticles and the ratio λ of the dipole–dipole interaction energy of two contacting particles to the thermal energy $k_B T$ [5]. These two dimensionless parameters are given as follows:

$$\phi = \frac{N}{V}\frac{\pi d_{\mathrm{p}}^3}{6} \tag{1}$$

$$\lambda = \frac{m^2}{4\pi\mu_0 k_{\mathrm{B}} T d_{\mathrm{p}}^3} \tag{2}$$

With respect to the fact that the suspended magnetic nanoparticles may aggregate under the influences of all the acting forces or potentials and there may exist some particle clusters, the conception of magnetic aggregation is put forward to deal with the interaction between two adjacent clusters or between the particles located in two adjacent lattices. For this purpose, the magnetic dipole moment of a cluster aggregation can also be considered as its magnetization and is treated with Weiss' theory [13]. A single-domain nanoparticle is subjected to an effective field instead of the applied field:

$$H_{\mathrm{e}} = H + H_{\mathrm{inter}} \tag{3}$$

where $H_{\mathrm{inter}} = \omega M$, the Lorentz value ω is equal to 1/3, H is the applied field, and M is the magnetization of cluster aggregation. Here H_{inter} is introduced to treat the nanoparticles distributed on a lattice as a cluster.

In ideal conditions, the cluster aggregation possesses the saturation magnetization as

$$M_{\mathrm{sat}} = \mu_0 M_{\mathrm{s,b}} V \tag{4}$$

where $M_{\mathrm{s,b}}$ denotes the bulk saturation magnetization of the material, and V is the volume of nanoparticle aggregation.

According to the terms of the Langevin function $L(\alpha) = \coth(\alpha) - 1/\alpha$ [5], one can obtain

$$M = M_{\mathrm{sat}} L(\alpha) \tag{5}$$

where $\alpha = mH_{\mathrm{e}}/k_{\mathrm{B}}T$.

Since the relation among expressions (3)–(5) is nonlinear, expression (5) is handled with Taylor's expansion near the point $M = M_{\mathrm{sat}}$ by ignoring the o[$(M - M_{\mathrm{sat}})$] term. Thus, the magnetic dipole moment of the nanoparticle aggregation in a lattice is calculated.

Thus, the ratio of dipole–dipole interaction energy of two contacting aggregation cluster to the thermal energy $k_{\mathrm{B}}T$ is similarly defined as:

$$\lambda' = \frac{M^2}{4\pi\mu_0 D^3 k_{\mathrm{B}} T} \tag{6}$$

where D is the equivalent diameter of the magnetic aggregation cluster. Here the aggregation cluster is considered as a sphere for the sake of simplicity.

3. Lattice-Boltzmann model form multicomponent system

Consider the motion of particles of S different components in a regular lattice in D-dimensional space. The population of the particles of the σth component with the velocity $\mathbf{e}_i$ at lattice site $\mathbf{x}$ and time t is denoted by $f_i^\sigma(\mathbf{x}, t)$, where $\{\mathbf{e}_i; i = 1, \ldots, b\}$ is the set of vectors pointing from $\mathbf{x}$ to its neighboring sites. In order to simulation the two-dimensional morphology and performance of the ferrofluid, one gets $S = 2$ and $b = 8$.

The evolution of $f_i^\sigma(\mathbf{x}, t)$ for a multicomponent system is described by the well-known lattice-Boltzmann equations:

$$f_i^\sigma(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) - f_i^\sigma(\mathbf{x}, t) = -\frac{1}{\tau_\sigma}\left(f_i^\sigma(\mathbf{x}, t) - f_i^{\sigma\mathrm{eq}}(\mathbf{x}, t)\right); \quad \sigma = 1, \ldots, S \tag{7}$$

where $\tau_\sigma = \eta_\sigma/\Delta t$ is the dimensionless collision–relaxation time constant of the σth component. On the right side, the Bhatnagar–Gross–Krook (BGK) single-relaxation time collision term [14] is adopted and the equilibrium distribution functions could be express as follows:

$$f_i^{\sigma,\mathrm{eq}} = \rho_\sigma w_i\left[1 + \frac{3}{c^2}(\mathbf{e}_i \cdot \mathbf{u}_\sigma) + \frac{9}{2c^4}(\mathbf{e}_i \cdot \mathbf{u}_\sigma)^2 - \frac{3}{2c^2}\mathbf{u}_\sigma \cdot \mathbf{u}_\sigma\right] \tag{8}$$

$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1, 2, 3, 4 \\ 1/36 & i = 5, 6, 7, 8 \end{cases} \tag{9}$$

The equilibrium distribution function $f_i^{\sigma,\mathrm{eq}}(\mathbf{x}, t)$ is selected to ensure that each of the components obeys the macroscopic Navier–Stokes equations. The following expressions describe the macroscaled quantities such as the mass density (or the number density) and the velocity of the σth component and the microscaled quantities defined on the basis of lattice sizes:

$$\rho_\sigma = \sum_i f_i^\sigma(\mathbf{x}, t) \tag{10}$$

$$\rho_\sigma \mathbf{u}_\sigma(\mathbf{x}, t) = \sum_i f_i^\sigma(\mathbf{x}, t)\mathbf{e}_i(\mathbf{x}, t) \tag{11}$$

These expressions are derived under the assumptions that there exist no internal or external forces and potentials acting on the particles, so that the total momentum of the particles of all components should be conserved by the scattering term (i.e. the collision term) at each lattice. For such a case, Shan and Doolen [14] assumed that the equilibrium velocity $\mathbf{u}_\sigma^{\mathrm{eq}}$ of each component is equal to a common velocity $\mathbf{u}^{\mathrm{eq}}$

$$\mathbf{u}^{\mathrm{eq}} = \sum_\sigma \frac{\rho_\sigma \mathbf{u}_\sigma}{\tau_\sigma} \Big/ \sum_\sigma \frac{\rho_\sigma}{\tau_\sigma} \tag{12}$$

For the actual multiphase fluid system such as a magnetic fluid, there exist some forces and/potentials acting on the particles. The impacts and influences from these forces and potentials cause an extra momentum change. As mentioned in a previous paper [12], the momentum supplement method and the modified collision-function

method are two main approaches to deal with the momentum variation induced by the forces and potentials. The first is the commonest and the most frequently used method by introducing an auxiliary momentum change $\tau_\sigma \mathbf{F}_\sigma \Delta t$ of the σth component to take the vector sum $\mathbf{F}_\sigma$ of all the acting forces and potentials into account. Thus, the equilibrium velocity is modified as

$$(\mathbf{u}_\sigma^{\mathrm{eq}})^* = \mathbf{u}^{\mathrm{eq}} + \tau_\sigma \mathbf{F}_\sigma \Delta t / m_\sigma \tag{13}$$

where m_σ is the mass density of the magnetic aggregation of the σth component.

It has been proven that formula (10) leads to a velocity field that is a solution of the Navier–Stokes equation. Here the kinetic viscosity v_σ of the σth component and the mean kinetic viscosity of the ferrofluid are respectively given as

$$v_\sigma = \frac{2\tau_\sigma - 1}{6}\frac{(\Delta x)^2}{\Delta t} \tag{14}$$

$$v = \frac{2\sum_\sigma \varphi_\sigma \tau_\sigma - 1}{6}\frac{(\Delta x)^2}{\Delta t} \tag{15}$$

where the concentration of each component $\varphi_\sigma = \rho_\sigma / \sum_\sigma \rho_\sigma$. Obviously, both expression (14) and (15) determine the relation between the kinetic viscosity, the relaxation constant, lattice length, and time step. For a real fluid system with a known kinetic viscosity, determination of the other parameters is confined by these expressions.

4. Forces and potentials in a ferrofluid

Among all the possible factors, as mentioned before, the mutual interaction among single particles and the action due to the external fields may be most important in controlling the phase behavior and morphology of the ferrofluid. Such actions can be described by a series of forces and potentials. Although the forces and potentials are considerably complicated, they can be sorted into two types: the continuous action and the transient impact. The gravitational force, Stokes drag force, the buoyancy, the magnetic force, and van der Waals attractive force belong to the first category and the Brownian force is of the second.

4.1. Interaction potentials

The ferrofluid structure is greatly affected by a number of acting forces and potentials. For the ferrofluid, the London-van der Waals attraction and the dipole–dipole interaction exist between the magnetic colloids. Generally, the van der Waals attraction potential between two adjacent spheres is expressed as [15]

$$\mathbf{V} = -\frac{A}{6}\left(\frac{2a^2}{L^2-4a^2} + \frac{2a^2}{L^2} + \ln\frac{L^2-4a^2}{L^2}\right) \tag{16}$$

where L is the distance between two adjacent particle cores and A is the Hamaker constant (approximately 4×10^{-20} J for iron oxides in a solvent).

For two adjacent spheres of radius a_s and a_p, Armin et al. [16] directly gave an expression for the van der Waals attraction force as follows:

$$\mathbf{F}_w = -\frac{A(16R)^3}{3(a_p+a_s)}\times\left[\frac{s}{(1+R)^2[s^2(1+R)^2-4(1-R)^2]^2}\right]e_r \tag{17}$$

where $s = \frac{2(L+a_p+a_s)}{a_p+a_s}$, $R = a_s/a_p$.

The dipolar interactions among the suspended magnetic nanoparticles and/or agglomeration clusters imply the interaction of fields produced by two magnetic particles and/or aggregations themselves and should be taken into account in the presence of an external magnetic field. Generally, the magnetic interaction between two magnetic nanoparticles and/or aggregation clusters with magnetic dipole moments $\mathbf{M}$ and $\mathbf{M}'$ at a distance r is given as

$$\begin{aligned} V_{MM'} &= -\mathbf{M}'\cdot\mathbf{H} \\ &= \frac{1}{4\pi\mu_0}\left[\frac{\mathbf{M}\cdot\mathbf{M}'}{r^3} - \frac{3}{r^5}(\mathbf{M}\cdot\mathbf{r})(\mathbf{M}'\cdot\mathbf{r})\right] \end{aligned} \tag{18}$$

For the uniform external magnetic field, the magnetic force induced by the external field is equal to zero. However, there still is a force acting on each particle as a result of the sum of the magnetic fields of all the other particles in the surrounding carrier liquid [17]. This internal force induced by such magnetic dipole moments potential is expressed as

$$\begin{aligned} \mathbf{F}_{\mathbf{MM}'} &= -\nabla V_{MM'} \\ &= -\frac{3}{4\mu_0\pi r^4}[(\mathbf{M}\cdot\mathbf{M}') - 3(\mathbf{M}\cdot\mathbf{r}_0)(\mathbf{M}'\cdot\mathbf{r}_0)]\mathbf{r}_0 \end{aligned} \tag{19}$$

where $\mathbf{r}_0$ denotes a unit vector.

These potentials are originally three dimensional. For the sake of simplicity, one may assume that they are applicable to the two-dimensional problem.

4.2. Other internal forces and external force

The other internal and external forces may include the Brownian force, drag force, gravitational force and buoyant force. All these actions also lead to momentum change inside the system.

Stokes' law is applied to describe the drag force due to the slip velocity difference $\Delta\mathbf{u}$ between the aggregation cluster and the carrier fluid as follows:

$$\mathbf{F}_D = -6\pi\mu a\Delta\mathbf{u} \tag{20}$$

Since the lattice-Boltzmann method assumes that the particles of the fluid are distributed in all lattices and the particle distribution in a given lattice possesses the same features, one may equate this particle distribution in the lattice as a fictitious particle while handling the drag force.

The sum of the buoyant force and the gravitational force is simply expressed as

$$\mathbf{F}_{\mathrm{H}} = \frac{4}{3}\pi a^3 g \Delta\rho \tag{21}$$

As for the irregular Brownian force, it can be considered as the comprehensive effect of the actions exerted by the surrounding fluid molecules. The Brownian force will lead to abrupt alteration of both velocity magnitude and direction of suspended particles or clusters. This random uncorrelated force statistically satisfies

$$\langle \mathbf{F}_i(t) \rangle = 0 \tag{22}$$

$$\langle \mathbf{F}_i(t)\mathbf{F}_j(t') \rangle = C\delta_{ij}\delta(t-t') \tag{23}$$

where i and j denote the components in the Cartesian coordinates, $\delta(t-t')$ is the Dirac function, C is a constant.

Since Brownian motion is generally simulated as a Gaussian white-noise process, the algorithm for simulating the Brownian force is similar to that for generating a white noise process modeled as a Gaussian white noise process [18],

$$\mathbf{F}_{\mathrm{B}} = \varsigma\sqrt{\frac{12\pi a\mu k_{\mathrm{B}}T}{\Delta t}} \tag{24}$$

where the parameter ς is a Gaussian random number with zero mean and unit variance.

The total force as $\mathbf{F}$ acting on the ferrofluid system is defined as the vector sum of all these forces, so that the extra momentum change induced by these internal and external forces is obtained as $\Delta\mathbf{P} = \mathbf{F}\tau_\sigma\Delta t$. Thus, the new equilibrium velocity is determined by the modification expression (13).

5. Results and discussion

The above-derived model can be used to investigate the structure of the magnetic particles suspended in a carrier liquid and simulate the morphology of the ferrofluid. The two-dimensional numerical simulations are

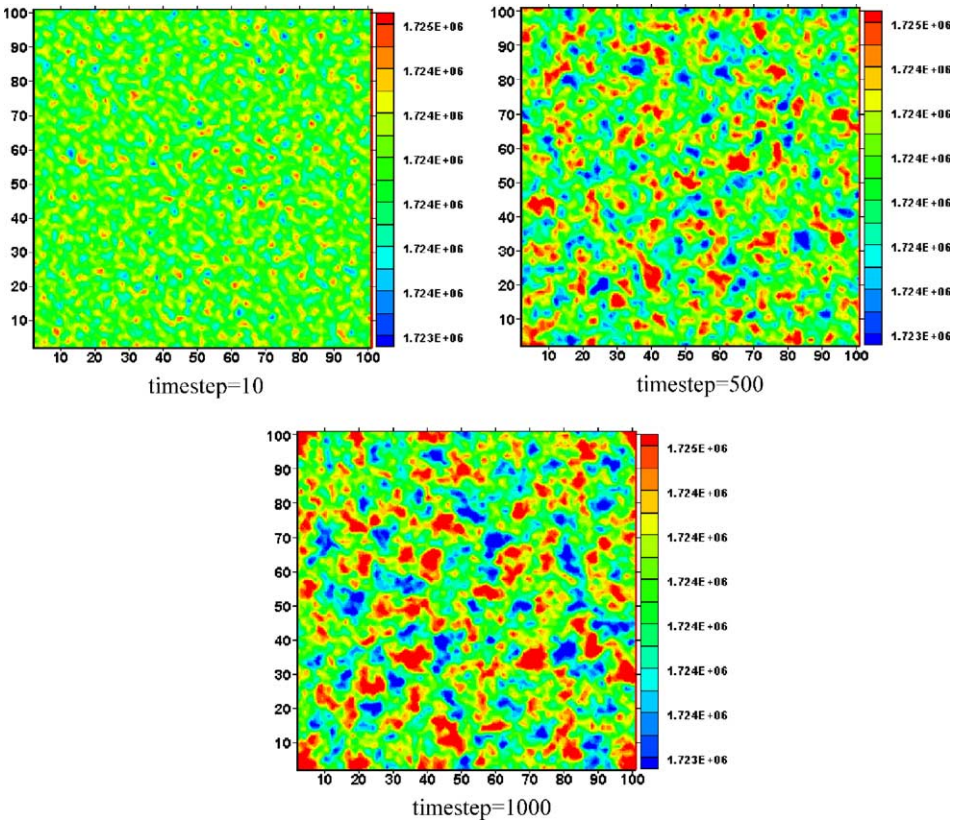

Fig. 1. Distribution of the particles d in the absence of an external magnetic field.

performed in a region consisting of 102×102 lattice grids, with periodic boundary conditions imposed on the x-axis and y-axis. Additional lattice sites are required at each end of the simulation region to implement the boundary conditions. The nominal diameter of the suspended Fe_3O_4 nanoparticles is 10 nm and the volume fraction of the solid magnetic particles is 10%. Since the time step Δt is set to be 10^{-7} s and τ_σ is set to be equal to 0.8 which is assumed to be the same for both components to get the correct statistical result, the spatial lattice length is determined with expression (14) or (15). It is assumed that the magnetic nanoparticles are evenly distributed all the lattices at the initial state.

Fig. 1 shows the distribution structures of the magnetic nanoparticles suspended in the carrier liquid whose the temperature is 298 K in the absence of an external magnetic field, in which the vertical coordinate on the right-hand side denotes the number density of the particles. It can be found that when the macroscopic flow velocity of the ferrofluid is zero, the nanoparticles tend to flocculate and the aggregation becomes more evident as the time increases. The Brownian force becomes the primary reason for keeping the suspended nanoparticles in random motion that provides a large probability of nanoparticle collision. Due to the sophisticated actions of various forces and potentials the suspended nanoparticles may tend to aggregate or flocculate, and then aggregation clusters may form. The larger sizes of nanoparticle clusters accelerate the sedimentation process. On the other hand, the thermal kinetic motion will break stable structures of the clusters, so that the clusters will be in an unstable state and aggregation and breakup of the clusters will coexist, which makes the distribution structure of the suspended nanoparticles more irregular.

Another example of the magnetic nanoparticle distribution in the presence of a perpendicular uniform field of 6×10^4 A m^{-1} is illustrated in Fig. 2 with the parameter $\lambda' = 4970$. Compared with Fig. 1, it is evident that the distribution structure of the suspended magnetic nanoparticles under the effect of the external magnetic field quite differs from that corresponding to no applied magnetic field. Long chainlike structures of the magnetic nanoparticles along the direction of the applied magnetic field form and such structures become more stable and clearer with increasing time. This phenomenon can be explained by the mechanism that the magnetic moment of the suspended magnetic nanoparticles quickly turns and remains identical to the direction of the applied field. Interaction potentials of these particles make the particles form chainlike structures along the mag-

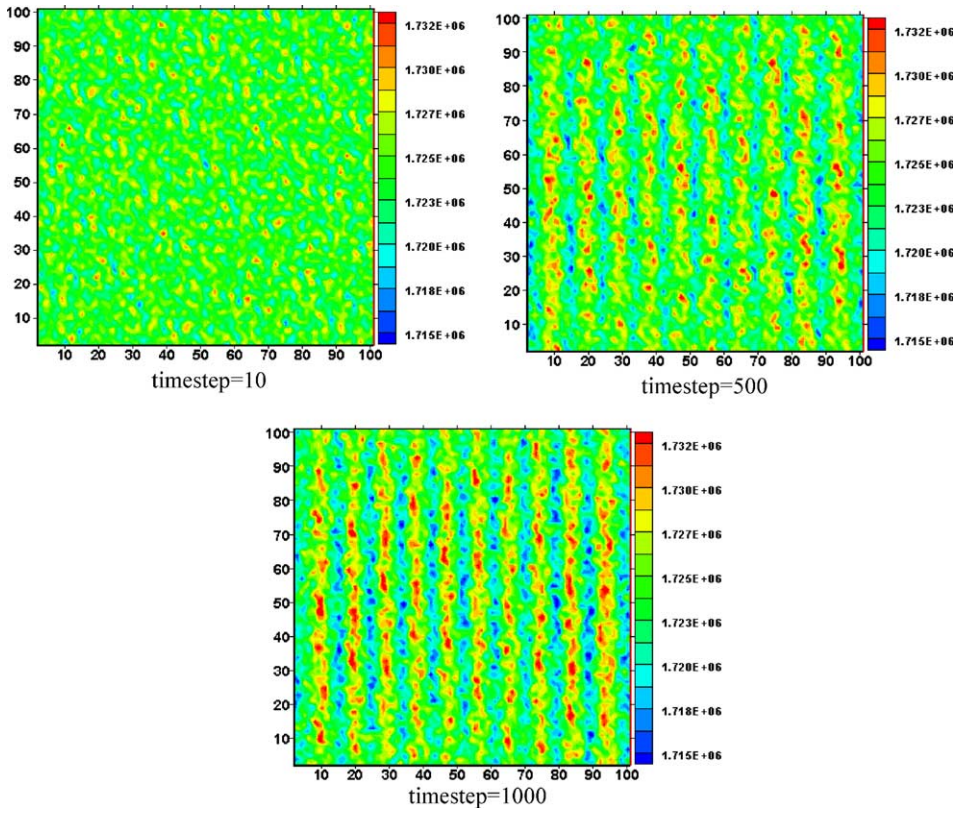

Fig. 2. Distribution of the particles under a uniform perpendicular field.

netic field. The Brownian motion may break larger clusters into smaller segments and tends to make the particles in irregular arrangements rather than along the direction of the external field, which will reduce the magnetization ability of the ferrofluid.

It is expected that in the presence of an external magnetic field, the dipole–dipole interaction energy and the thermal energy are two of the dominant factors for controlling the morphology and magnetization ability of the ferrofluid. As mentioned before, the magnitude of parameter λ' indicates the comprehensive effect of both these two types of energy on the microscale structure of the ferrofluid. For example, consider the case that the diameter of a magnetic aggregation cluster is 100 nm, the bulk saturation magnetization of the material is 4.8×10^5 A/m, and the fluid temperature is 298 K, one can get $\lambda' = 1530$. A higher value of λ' means a stronger effect of the dipole–dipole magnetic energy. Note that the parameter λ' increases with the magnetization intensity and decreases with the fluid temperature.

Fig. 3 provides some comparison examples about the distribution structures of the suspended magnetic nanoparticles corresponding to different values of the parameter λ' after the same timestep (timestep = 1000). As shown, the morphology of the ferrofluid system varies from the random distribution of the suspended magnetic nanoparticles to short clusters or string-like alignments along the direction of the external applied magnetic field with increasing λ'. According to numerical simulations, the dependence of magnetic nanoparticle distribution on an external magnetic field is rather weak if $\lambda' < 4029$. In such cases, the Brownian force due to the thermal impulse plays a preponderant role on the arrangement structure of the suspended magnetic nanoparticles as well as the distribution of the magnetic moment. But if $\lambda' \geqslant 4577$, the nanoparticles appear in a chainlike arrangement along the external field and short-chain aggregation clusters emerge.

The effects of a horizontal magnetic field on the distribution structures of the suspended magnetic nanoparticles are illustrated in Fig. 4, in which the other parameters remain the same as those in Fig. 3. Compared with the simulation results corresponding to the vertical magnetic field, the horizontally applied magnetic field leads to a quite different morphology of the ferrofluid. Of course, the distribution structures of the suspended nanoparticles depend upon the integrated effect of all the forces and potentials acting on the ferrofluid system. Such effects are distinctly indicated by two extreme cases (as shown in Fig. 4): one is that the

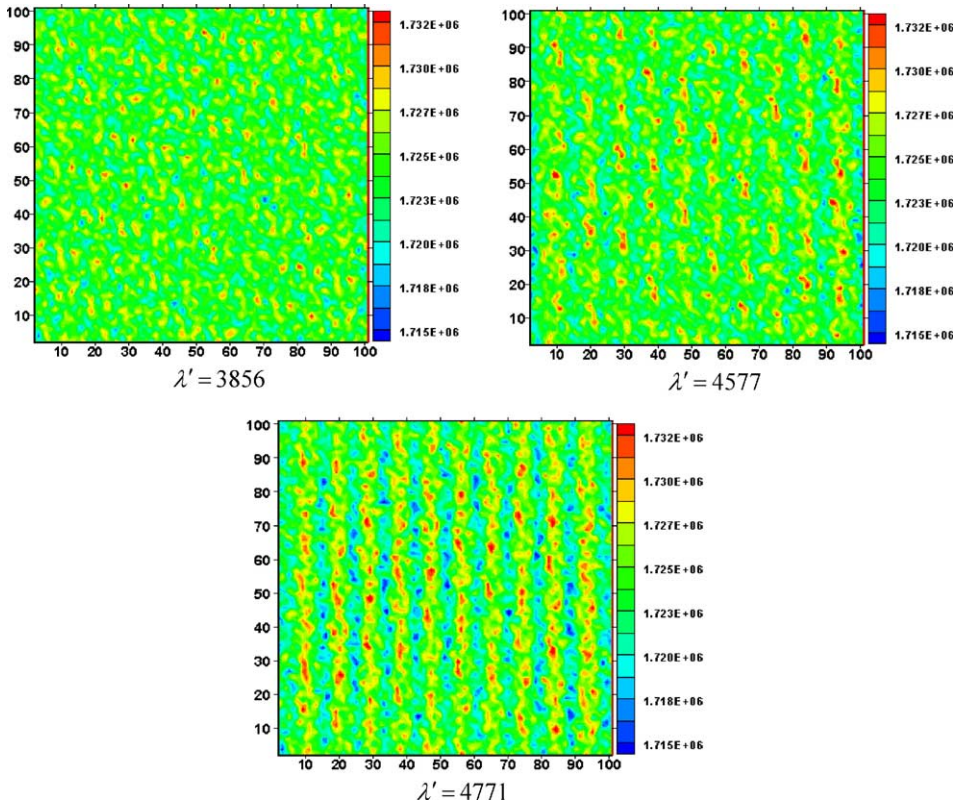

Fig. 3. Distribution of the particles with an applied uniform perpendicular field corresponding to different λ'.

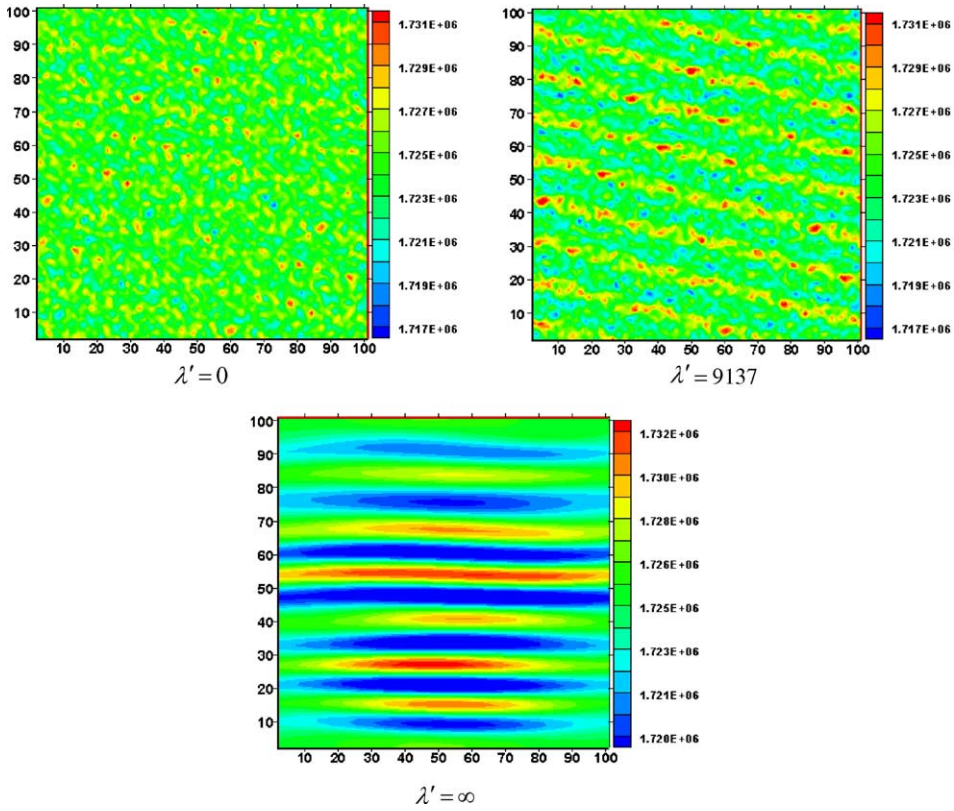

Fig. 4. Distribution of the particles with an applied uniform horizontal field corresponding to different λ'.

dipole–dipole interaction among the magnetic nanoparticles is ignored ($\lambda' = 0$) and the other is that the effect of the Brownian force is neglected ($\lambda' = \infty$). In the first case, the Brownian force may play a dominant role in the distribution of the nanoparticles, so that the morphology appears as a random state. As the value of parameter λ' increases, the effect of the external magnetic field through the dipole–dipole interaction becomes more important. When $\lambda' = \infty$ and the Brownian force is small enough to be neglected, the magnetic moments of the suspended magnetic nanoparticles turn to the direction of the applied magnetic field and the nanoparticles horizontally appear in a chainlike arrangement along the external horizontal magnetic field. The intermediate states between these extreme cases reveal the competitive and opposite functions of the Brownian force and the applied magnetic field. The Brownian force always promotes the random motion of the suspended nanoparticles and tries to prohibit the nanoparticles to be aligned in the external magnetic field, so it will reduce the magnetization ability of the ferrofluid.

It should be mentioned that the D2Q9 model has been introduced for two-dimensional simulation of the morphology of a magnetic fluid. In principle, the above-described approach can directly be extended to three-dimensional simulation. For this purpose, the suitable density distribution functions of artificial particles corresponding to the three-dimensional structures such as the D3Q15 or D3Q19 model should be substituted for the D2Q9 model and the relevant variations involved in relations between the microscopic parameters and the macroscopic ones should be taken into account.

6. Conclusions

In this paper, a lattice-Boltzmann model for simulating the distribution structure of the suspended magnetic nanoparticles and the morphology of the ferrofluid has been developed. Some possible acting forces and potentials such as the gravitational force, the Stokes drag force, the Brownian force, van der Waals attraction potential, and the dipole–dipole interaction potential have been incorporated into the model. The momentum supplement method has been used to deal with the momentum variation induced by the vector sum of all these forces and potentials by introducing an auxiliary momentum change of the σth component. By means of the proposed model the structure of the ferrofluid at the mesoscale level can be simulated without the limitation

of nanoparticle number, compared with the direct numerical simulation method of a flow system.

Several examples have been computed and the numerical simulation results have revealed the effects of the forces and potentials on the distribution microstructure of the magnetic nanoparticles. Among all the forces and potentials the thermal fluctuation force and the external allied magnetic field are two dominant factors of controlling the morphology of the ferrofluid. Furthermore, they exert quite opposite effects on the aggregation clusters structures and the magnetization ability of the ferrofluid. The applied magnetic field enhances the tendency of coalignment with the field direction and aggregation of the suspended magnetic nanoparticles, but the Brownian force keeps the nanoparticles in random motion and suppresses the effect of the external magnetic field.

Acknowledgment

This work was supported by the National Natural Science Foundation of China (Grant no. 50376023 and 50436020).

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