DIRECT NUMERICAL SIMULATION OF PARTICLE BROWNIAN MOTION IN A FLUID WITH INHOMOGENEOUS TEMPERATURE FIELD

by

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In this work the fluctuating-lattice Boltzmann method was adopted to numerically investigate the Brownian motion of particles in a fluid with inhomogeneous temperature field. It has been found that the Brownian particles are preferential to randomly move into a cold fluid area. Once the particles go into the cold area, the boundary between the hot fluid and cold fluid acts like a temperature barrier, preventing the particles from going out. Most important of all, the Brownian particles can be captured or collected by the cold fluid area if the temperature of cold fluid is lower than a critical value. In addition, the dependence of this critical value on the fluid viscosity is studied.

Key words: Brownian motion, nanoparticle, preferential motion, lattice Boltzmann method

Introduction

Particles suspended in fluids experience a random force due to the thermal fluctuations in the fluid around them in addition to the average hydrodynamic force. Brownian motion may take place for those sub-micro/nanoscale particles. For many applications in microsystems, the ability to control and measure temperature inside microfluidic devices is critical since temperature often affects biological or chemical processes. It has been shown that the well-defined temperature dependence of the Brownian motion of nanoparticles could be used to present a temperature measurement technique which offers several benefits over existing methodologies [1, 2]. Brownian particle can be adopted to measure the local viscoelastic response of soft materials [3] or the topography of a surrounding polymer network [4]. The motion of a Brownian probe can also be used to characterize mechanical properties of molecular motors by analyzing the particle's trajectory [5]. Moreover, the biased Brownian motions or rectified Brownian motions, induced by an energy source [6] or by broken spatial reflection symmetry [7], provide a very effective technique for particle separation. Furthermore, it has been demonstrated [8, 9] that nanoparticles in a conventional base fluid, known as nanofluids, tremendously enhance the heat transfer characteristics of the original fluid. At the same time, study [10] has declared that Brownian motion is a key mechanism governing the thermal behavior of nanofluids.

Due to its importance in engineering applications, there has always been a great deal of interest in developing algorithms that can provide a better understanding of particle Brownian motion. Lin *et al.* [11] studied the constrained Brownian motion of a sphere be-

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tween two walls through an experimental work. The perpendicular and parallel diffusion coefficients of the sphere were presented and evaluated [11]. The same problem was also studied by Benesch et al. [12] who used the method of reflection. Iwashita et al. [13] investigated the effect of fluid inertia on the short-time motion of Brownian particles by using the direct numerical simulations. They [13] found that the mean square displacements (MSD) in the vorticity direction grows rapidly in time and with increasing particle volume fraction. In addition, their results indicated that the particles are no more diffusive due to the shear-induced ordering for volume fraction up to 0.5. Similarly, Uma et al. [14] used a fluctuating hydrodynamics approach to study the Brownian motion of a nanoparticle in a fully developed Poiseuille flow. They compared the translational and rotational velocity autocorrelation function (VACF) and MSD with analytical and experimental results. They also verified the equipartition theorem for a Brownian particle in Poiseuille flow for a range of low Reynolds numbers. Recently, Radiom et al. [15] conducted an experiment to measure the hydrodynamic interactions between two Brownian spheres at low Reynolds numbers, to check the effect of fluid inertia. They [15] showed that the hydrodynamic interaction between the Brownian particles can be predicted by the analytical expressions that neglect the inertia of the fluid when the interparticle separation is less than twice the thickness of the Stokes layer. On this basis, they [15] suggested a way to predict when fluid inertial effects can be ignored by including the gap-width dependence into the frequency number. More recently, Mo et al. [16] studied the Brownian motion of a sphere in the vicinity of a plane wall, showing the effect of wettability on the statistical properties of particle motion. Cichocki et al. [17] performed a theoretical analysis of the Brownian motion of a particle with an arbitrary shape. They [17] derived analytical expressions for the time-dependent cross-correlations of the Brownian translational and rotational displacements. Jahanshahi et al. [18] studied the dynamics of a Brownian circle swimmer in an external harmonic potential and found a resonance situation for the maximum escape distance as a function of the various frequencies in the system. Dessup et al. [19] investigated the Brownian motion of a chain of interacting particles in a confining channel. They [19] revealed that the mean squared displacement can be larger in a corrugated channel than in a smooth one due to the corrugations and their fluctuations.

It is well known that the Brownian motion of particles is very sensitive to fluid temperature. The higher the fluid temperature is, the stronger the Brownian motion of particles is. Undoubtedly, the Brownian motion is isotropic if the fluid temperature is homogeneous everywhere, which leads to a totally random movement of particles in the fluid. However, the random movement of particles may be changed if the fluid temperature is inhomogeneous. For instance, the Brownian motion may become biased if there are hot fluid and cold fluid in a flow field because the thermal fluctuations are determined by the temperature. Is there a preferential motion for the Brownian particles under this condition? How does a Brownian particle cross the boundary between hot fluid and cold fluid? What does this boundary act like? To answer these questions, a systematic study is needed to better understand the feature of Brownian motion in an inhomogeneous environment. However, to our knowledge this issue has not been investigated so far. This motivates the present work.

The most accurate approach to simulate particle Brownian motion is the fluctuating hydrodynamics method, which was proposed by Landau *et al.* [20]. In this approach, the thermal fluctuations of fluid molecules, the origin of the Brownian motion, are modeled by adding a random stress tensor to the Navier-Stokes equations. Solving the fluctuating hydrodynamic equations coupled with the equations of particle motion (Newton's Second law of mo-

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tion) result in the Brownian motion of particles. As a direct numerical simulation scheme, there is no need to add a random force term in the equations of particle motion since random fluctuations are applied directly to the particles, which differs from the Langevin dynamics. So far the lattice Boltzmann method (LBM) has become a useful tool for simulating particulate flows [21-23]. The bounce-back (BB) rule [24] was first introduced to impose no-slip boundary conditions in LBM. The combination of LBM and BB boundary condition was proved to be robust and efficient in the simulations of particulate flows with large number of particles. Application of LBM coupled with fluctuating hydrodynamics to simulate particle Brownian motion was first proposed by Ladd [25], which is performed by adding a fluctuating term in the lattice Boltzmann equation. Nie *et al.* [26] also proposed a fluctuating-lattice Boltzmann method (FLBM) based on the single-relaxation-time model, which can successfully account for the short-time motion and deal with particles of irregular shape in a straightforward manner. To better understand the effect of the fluid temperature we aim to investigate the Brownian motion of particles in an inhomogeneous circumstance through the FLBM in this work [26].

Numerical method

The fluid flow is solved by the FLBM [26]. The discrete lattice Boltzmann equations of single-relaxation-time model are described:

$$f_i(\boldsymbol{x} + \boldsymbol{e}_i \Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = -\frac{1}{\tau} \Big[f_i(\boldsymbol{x}, t) - f_i^{(eq)}(\boldsymbol{x}, t) \Big] + f_i^{(B)}(\boldsymbol{x}, t)$$
(1)

where $f_i(\mathbf{x}, t)$ is the distribution function on the *i*-direction discrete velocity $\mathbf{e}_i, f_i^{(eq)}(\mathbf{x}, t)$ – the equilibrium distribution function, Δt – the time step, τ – the relaxation time, $f_i^{(B)}(\mathbf{x}, t)$ – the stochastic term representing the thermal fluctuations, which is related to the fluctuating stress in the Navier-Stokes equations [26].

The fluid density, ρ , and velocity, \boldsymbol{u} , are determined by the distribution function:

$$\rho = \sum_{i} f_{i}, \quad \rho \boldsymbol{u} = \sum_{i} f_{i} \boldsymbol{e}_{i}$$
(2)

For the 2-D D2Q9 lattice model used here, the discrete velocity vectors are:

$$\boldsymbol{e}_{i} = \begin{cases} (0,0), & \text{for } i = 0\\ (\pm 1,0)c, \ (0,\pm 1)c, & \text{for } i = 1 \text{ to } 4\\ (\pm 1,\pm 1)c, & \text{for } i = 5 \text{ to } 8 \end{cases}$$
(3)

where $c = \Delta x / \Delta t$, Δx is the lattice spacing. The equilibrium distribution function is chosen:

$$f_{i}^{(\text{eq})}(\mathbf{x},t) = w_{i}\rho \left[1 + \frac{e_{i}u}{c_{s}^{2}} + \frac{(e_{i}u)^{2}}{2c_{s}^{4}} - \frac{uu}{2c_{s}^{2}}\right]$$
(4)

where $c_s^2 = c^2/3$ and c_s is the speed of sound, and the weights are set to be $w_0 = 4/9$, $w_{1-4} = 1/9$ and $w_{5-8} = 1/36$.

As illustrated by Nie *et al.* [26], the stochastic term is related to the fluctuating stress in the following way:

$$\sigma_{\alpha\beta}^{(B)} = -\tau \sum_{i} f_{i}^{(B)} e_{i\alpha} e_{i\beta}$$
⁽⁵⁾

According to the fluctuation-dissipation theorem, $\sigma_{\alpha\beta}^{(B)}$ has the following property [20]:

$$\left\langle \sigma_{\alpha\beta}^{(B)} \right\rangle = 0$$

$$\left\langle \sigma_{\alpha\beta}^{(B)} \left(\mathbf{x}, t \right) \sigma_{\gamma\delta}^{(B)} \left(\mathbf{x}', t' \right) \right\rangle = 2k_{B}T \mu \left(\delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma} - \frac{2}{3} \delta_{\alpha\beta} \delta_{\gamma\delta} \right) \delta_{\mathbf{x}\mathbf{x}'} \delta_{tt'}$$
(6)

where $\langle \rangle$ denotes averaging over an ensemble, k_B – the Boltzmann constant, T – the temperature of the fluid, and μ – the dynamic viscosity of the fluid. The fluctuating stress is sampled from a Gaussian distribution with zero mean and a given variance of $2k_BT\mu$. As shown by Nie *et al.* [26], the following Navier-Stokes equations can be recovered from the lattice Boltzmann equations through a Chapman-Enskog expansion:

$$\partial_t \rho + \partial_\alpha \left(\rho u_\alpha \right) = 0 \tag{7a}$$

$$\partial_t(\rho u_{\alpha}) + \partial_{\beta}(\rho u_{\alpha} u_{\beta}) = -\partial_{\alpha} p + v \partial_{\beta} \Big[\partial_{\alpha}(\rho u_{\beta}) + \partial_{\beta}(\rho u_{\alpha}) \Big] + \partial_{\beta} \sigma^f_{\alpha\beta}$$
(7b)

Then the kinematic viscosity of fluid is given by $v = c_s^2(\tau - 0.5)\Delta t$. In this work we assume the stochastic term $f_i^{(B)}(\mathbf{x}, t)$ to be the following form to make sure of the conservation of mass and momentum:

$$f_{0}^{(B)} = 0$$

$$f_{1}^{(B)} = f_{3}^{(B)} = \frac{1}{2\tau} \sigma_{yy}^{(B)}$$

$$f_{2}^{(B)} = f_{4}^{(B)} = \frac{1}{2\tau} \sigma_{xx}^{(B)}$$

$$f_{5}^{(B)} = f_{7}^{(B)} = -\frac{1}{4\tau} \left[\sigma_{xx}^{(B)} + \sigma_{yy}^{(B)} + \sigma_{xy}^{(B)} \right]$$

$$f_{6}^{(B)} = f_{8}^{(B)} = -\frac{1}{4\tau} \left[\sigma_{xx}^{(B)} + \sigma_{yy}^{(B)} - \sigma_{xy}^{(B)} \right]$$
(8)

In the simulations, the momentum-exchange scheme proposed by Ladd [24] was used to calculate the force and torque experienced by the particles. Then the motion of particles can be updated by solving the Newton's equations.

Validation

In this work, the Brownian motion of 16 particles in a periodic domain was simulated to validate the present method. In the simulations only the hydrodynamic force was considered. The periodic domain is set to be 256×256 . The density of the fluid is fixed at $\rho = 1$ and the non-dimensional relaxation time $\tau = 0.65$, which leads to the viscosity of the fluid $v = (2\tau - 1)/6 =$ = 0.05. The radius of particle is a = 4.5. The solid/fluid density ratio is fixed at $\rho_s/\rho = 11$. In order to determine the magnitude of the fluid fluctuation, the temperature of fluid is chosen as $T = 10^{-4}$ and the Boltzmann constant is $k_B = 1$. It should be stated that all the aforementioned parameters are in lattice units.

The instantaneous flow at different times is shown in fig. 1, along with the Brownian particles. The time is normalized through $t' = tv/a^2$. In fig. 1, the thermal fluctuations are clearly illustrated by the magnitude of fluid velocity |u| (normalized by v/a), which are visually disordered in space and time, representing the random molecular motion of the fluid. This is the

origin of the Brownian motion of particles, resulting from the essence of the present FLBM, which is different from the Langevin dynamics. As shown in fig. 1, the particles tend to spread out with time as they undergo Brownian motion, displaying the classical motion of Brownian diffusion. In addition, it is worth stating here that the rotation of particles can be realized in the present simulations, as shown in fig. 1. This is one of the advantages of fluctuating hydrodynamics method [20] over the Langevin dynamics.



Figure 1. Instantaneous flow (normalized magnitude of fluid velocity, |u|a/v, the same as below) of Brownian motion at different times; (a) t' = 12.4, (b) t' = 123.5, (c) t' = 246.9, (d) t' = 493.8, (e) t' = 987.7, and (f) t' = 1975.3; the white arrow on each particle is used to visually track its rotation with horizontal orientation at the beginning (the same as below)

It has been theoretically demonstrated that thermal equilibrium between the Brownian particle and the surrounding fluid molecules will reach and that an equi-partition of energy for each degree of freedom will be observed, which can be described:

$$\left\langle U^{2}(t)\right\rangle = \frac{k_{B}T}{M}, \quad \left\langle \Omega^{2}(t)\right\rangle = \frac{k_{B}T}{J}$$
(8)

where U and Ω refer to the translational velocity and rotational velocity of particle, respectively. The M and J are the mass and moment of inertia of particle, respectively. The mean square of U and Ω are characterizing the particle temperatures of translational motion and rotational motion, respectively. They are normalized by k_BT/M and k_BT/J in fig. 2, respectively. The particle temperatures are within 5% accuracy compared to the effective temperature of fluid, as one can see in fig. 2, which indicates that there is thermal equilibrium between the Brownian particles and the surrounding fluid.

The long-time tails are fundamental to help understanding the physics of Brownian motion. Figure 3 shows the translational and rotational VACF of particles. All the results are normalized by their initial values, *i. e.* the values at t = 0. As demonstrated by Alder *et al.* [27] and Ailawadi *et al.* [28], the translational and rotational VACF of a disk undergoing Brownian motion have power-law decays over long times that are t^{-1} and t^{-2} , respectively, which is different from the exponential decay predicted by Langevin dynamics. As shown in fig. 3, the similar long-time tails are observed for the circular particles in the present simulations, which is consistent with the previous results [27, 28].



Figure 2. Time history of mean squares of the translational and rotational velocity of Brownian particles, which are normalized by k_BT/M and k_BT/J , respectively



Figure 4. Schematic diagram of the present problem



Figure 3. Translational and rotational VACF of Brownian particles, which are normalized by $\langle U^2(0) \rangle$ and $\langle W^2(0) \rangle$, respectively

Results and discussion

First of all, the Brownian motion of a single particle in a fluid with inhomogeneous temperature is numerically investigated. As shown in fig. 4, a particle with radius *a* is freely moving resulted from thermal fluctuation of the surrounding fluid. The size of computational domain is $L \times L$. We assume that there is a circular area with radius, R, inside which the fluid is cold. The temperature is denoted as $T_{\rm c}$. The hot fluid with temperature, $T_{\rm h}$, fills with the rest of domain. For simplicity we choose no-slip boundary conditions on all four fixed walls of the domain, as shown in fig. 4. In all simulations, the parameters are fixed at a = 4.5, $T_{\rm h} = 1.0 \cdot 10^{-3}$, and $\rho_s / \rho = 11$. For a single particle the domain is set to be L = 14a and R = 3.5a.

In addition, the non-dimensional relaxation time is fixed at $\tau = 0.6$ unless otherwise stated. The particle is initially placed in the center of the domain.

Figure 5 shows the instantaneous flow of particle Brownian motion at different times. Four kinds of cold temperature are taken into account, *i. e.* $T_c = 1.0 \cdot 10^{-3}$, 5.0×10^{-4} , $1.0 \cdot 10^{-4}$ and $5.0 \cdot 10^{-5}$ (from top to bottom). For the results of $T_c = 1.0 \cdot 10^{-3}$, the root mean square (RMS) of fluid velocity is homogeneous everywhere because there is no temperature difference in the fluid. However, things are different for other results. According to eq. (6), for constant viscosity the magnitude of thermal fluctuation of fluid molecule is determined by the fluid temperature,



Figure 5. Instantaneous flow of Brownian motion at different times; (a) t' = 16.4, (b) t' = 164.6, (c) t' = 658.4 and (d) t' = 1646.1; the values of T_c are $1 \cdot 10^{-3}$, $5 \cdot 10^{-4}$, $1 \cdot 10^{-4}$ and $5 \cdot 10^{-5}$, from top to bottom

suggesting that low temperature leads to slow thermal motion. By displaying the RMS of fluid velocity, a cold temperature zone is observed in the central area, which is more obvious when decreasing the value of T_c , as we can see in fig. 5. When there is no cold fluid (the case of $T_c = 1.0 \cdot 10^{-3}$), the particle is randomly moving in the whole domain. However, the particle will experience a small Brownian force once it enters the cold temperature area, leading to the fact that the motion of particle is slowed down in this area. Furthermore, numerical simulations also indicate that there is more trend for the particle to enter the cold temperature area when the value of T_c is lower. Most important of all, it is found that the particle will stay in the cold area if T_c is low enough, which is seen for the cases of $T_c = 1.0 \cdot 10^{-4}$ and $T_c = 5.0 \cdot 10^{-5}$.

As shown in fig. 5, in view of the value of R = 3.5a the cold temperature area is very small. Even so, the particle seems to stay in this area all the time. The boundary between the hot fluid and cold fluid acts like a temperature barrier, which prevents the particle from entering the hot fluid area. The reason behind this is that the particle will experience much stronger collisions due to the hot fluid molecules once it goes across the boundary. These collisions act as a stronger repulsive force to prevent the particle moving forward.

In order to better address this issue, we present the trajectories of particle during $t' = 0 \sim 2300$ for different values of T_c in fig. 6. The co-ordinates are normalized through x' = x/a and y' = y/a. The effect of T_c on the particle Brownian motion is significant, as one can see from the figure. When decreasing the value of T_c the particle is likely to move around the central area, *i. e.* the cold area. In particular, the trajectory is nearly sited at the cold area for the case of $T_c = 1.0 \cdot 10^{-4}$, which further indicates that the particle is kept from entering the hot fluid area.



Figure 6. Trajectories of particle Brownian motion during t' = 0~2300 for different values of T_c ; (a) 1·10⁻³, (b) 4·10⁻⁴, and (c) 1·10⁻⁴; the blue circle represents the initial position of Brownian particle

Figure 7 shows the trajectories of particle for $T_c = 1 \cdot 10^{-4}$ at different initial positions. As one can observe, though the particle starts to move from different position (even at the hot fluid area), it enters the cold fluid area and stays there eventually. This is interesting because it provides a new way to capture or collect the Brownian particles (sub-micro particles or nanoparticles) in a fluid. If the fluid temperature is the same everywhere, the Brownian motion of particles is random but isotropic, which leads to a homogeneous distribution of particles. However, the Brownian particles will exhibit a preferential motion if there is temperature difference in the fluid. In addition, there is an increasing trend for the particles to move towards the cold fluid area with decreasing temperature. This makes it possible that the Brownian can be captured by the cold temperature area somewhere in the fluid.

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Figure 7. Trajectories of particle Brownian motion during $t' = 0 \sim 2300$ for $T_c = 1 \cdot 10^{-4}$ at different initial positions

In what follows we present another two cases to further illustrate the influence of temperature barrier. The first case is depicted in fig. 8, showing the instantaneous flow (at t' = 2469.1) of Brownian motion of 36 particles for different values of T_c . The parameters are set to be L = 16a, R = 10a, and $\tau = 0.6$. In comparison with the case of single particle, fig. 5, similar results can be observed. The particles are randomly distributed in the whole domain when the fluid temperature is homogeneous ($T_c = 1 \cdot 10^{-3}$), as shown in fig. 8(a). Nevertheless, it is clear that the particles are preferential to stay in the central area when $T_c = 5 \cdot 10^{-4}$. In particular, all the particles will go into the central area eventually when the temperature is low enough, such as $T_c = 1 \cdot 10^{-4}$, as depicted in fig. 8(c). In other words, the cold area captures all the particles when they are randomly moving in the fluid.



Figure 8. Instantaneous flow of Brownian motion of 36 particles at t' = 2469.1 for different values of T_c ; (a) $T_c = 1 \cdot 10^{-3}$, (b) $T_c = 5 \cdot 10^{-4}$, and (c) $T_c = 1 \cdot 10^{-4}$

Figure 9 shows the instantaneous flow of Brownian motion of 36 particles for $T_c = 5 \cdot 10^{-5}$ at different times, which clearly illustrates how the cold area captures all the particles. At the beginning of the simulation, the particles are placed homogeneously over the computational domain, as one can see in fig. 9(a). In this case the temperature of the cold fluid is very low, resulting in very small thermal fluctuations in the central area. As a consequence, most of particles quickly go into the central area and do not leave, which is seen in fig. 9(c). Furthermore, it takes a much longer time for the rest of particles to be captured. The reason behind this is clear. There is not much room for these particles in the central area. When approaching this area, they are repelled due to the hydrodynamic interactions as well as particle collisions.



Figure 9. Instantaneous flow of Brownian motion of 36 particles for $T_c = 5 \cdot 10^{-5}$ at different times: (a) t' = 0.16, (b) t' = 164.6, (c) t' = 329.2, (d) t' = 658.4, (e) t' = 1316.9, and (f) t' = 2469.1

The second case is illustrated in fig. 10. The parameters are L = 32a, $\tau = 0.6$, and $T_c = 5 \cdot 10^{-5}$, and the number of particles is 100. A channel-like area of cold fluid is used in this case instead of a circular area. The results are similar to those shown in fig. 9.

The effect of fluid viscosity, v, is also investigated in this work. It is found that the effect of temperature barrier is decreasing when increasing v. This can be observed from fig. 11,



Figure 10. Instantaneous flow of Brownian motion of 100 particles for $T_c = 5 \cdot 10^{-5}$ at different times; (a) t' = 16.5, (b) t' = 329.2, and (c) t' = 1975.3

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Figure 11. Trajectories of particle Brownian motion ($T_c = 5 \cdot 10^{-5}$) for different viscosity; (a) v = 1/6, (b) v = 1/10, and (c) v = 1/30

which presents the trajectories of single particle for $T_c = 5 \cdot 10^{-5}$ for different fluid viscosity. Other parameters are the same to those of fig. 7. It is interesting to find that the effect of temperature barrier on the Brownian motion of particle is almost negligible for v = 1/6. The particle can hardly *feel* the boundary between the hot fluid and cold fluid in this case, even at the low temperature as $T_c = 5 \cdot 10^{-5}$. However, results show that there still exists a critical value of T_c (*i. e.* T_c^*) below which the particle can be captured.

To gain more insight into this issue, we carry out a large amount of simulations to obtain the critical value of T_c by varying the fluid viscosity (the relaxation time τ), under the same flow conditions. We summarize the results in fig. 12. As one can observe in the figure, the value of T_c^* decreases sharply as the viscosity increases (note the log-log scale), which indicates that very low temperature is needed to capture the nanoparticles when they are randomly moving in the fluid with large viscosity. Furthermore, a power-law relationship is observed between T_c^* and ν . The exponent value is found to be about -2.08 through the least square calculation.

Finally, it should be mentioned that the viscosity is kept constant for every single simulation in this work. In other words, the effect



Figure 12. Dependence of the critical value of T_c (*i. e.* T_c^*) on the fluid viscosity v

of fluid temperature on its viscosity is not taken into account. In general, the fluid viscosity decreases as the temperature increases. However, it is believed that there exist some fluids whose viscosity are not sensitive to the temperature. Therefore, the conclusion of this work still stands for these fluids. On the other hand, we believe that only the critical value of T_c may be different if we consider the effect of fluid temperature on its viscosity. Of course, to understand further the complex dynamics involved in this process, we intend to perform simulations with these kinds of effect. Also, 3-D situations, that is, the Brownian motion of spheres, will be considered in the near future.

Conclusion

In this work the previously developed FLBM was adopted to numerically investigate the preferential Brownian motion of particles in a fluid with inhomogeneous temperature field.

First of all, the method was validated by simulating the Brownian motion of 16 particles in a fluid with homogeneous temperature field. The computed translational or rotational velocity correlation function has a long-time tail, decaying at t^{-1} or t^{-2} at long times, which is consistent with the theoretical prediction. Then, the method was used to simulate the Brownian motion of particles in a fluid with high temperature and low temperature. Results show that the particles are preferential to randomly move into the cold fluid area. Most important of all, the particles go into the cold area and stay there eventually if the temperature of the cold area is low enough, irrespective of their initial positions. In other words, the cold fluid can capture or collect the Brownian particles. Once the particles enter the cold area, the boundary between hot fluid and cold fluid acts like a temperature barrier, which prevents the particles going out. Furthermore, there exists a critical value of cold fluid temperature, below which the particles can be captured. And this critical value decreases as the fluid viscosity increases.

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References

- Park, J. S., *et al.*, Temperature Measurement for a Nanoparticle Suspension by Detecting the Brownian Motion Using Optical Serial Sectioning Microscopy (OSSM), *Measurement Science and Technology*, *16* (2005), 7, pp. 1418-1429.
- [2] Chung, K., et al., Three-Dimensional in Situ Temperature Measurement in Microsystems Singu Brownian Motion of Nanoparticles, Analytical Chemistry, 81 (2009), 3, pp. 991-999
- [3] MacKintosh, F. C., et al., Microrheology, Current Opinion in Colloid & Interface Science 4, (1999), 4, pp. 300-307
- [4] Tischer, C., et al., Three-Dimensional Thermal Noise Imaging, Applied Physics Letters, 79 (2001), 23, pp. 3878-3880
- [5] Jeney, S., et al., Mechanical Properties of Single Motor Molecules Studies by Three-Dimensional Thermal Force Probing in Optical Tweezers, Chem. Phy. Chem., 5 (2004), 8, pp. 1150-1158
- [6] Dean Astumian, R., Thermodynamics and Kinetics of a Brownian Motor, Science, 276 (1997), 5314, pp. 917-922
- [7] Derenyi, I., et al., AC Separation of Particles by Biased Brownian Motion in a Two-Dimensional Sieve, Physical Review E, 58 (1998), 6, pp. 7781-7784
- [8] Keblinski, P., et al., Mechanisms of Heat Flow in Suspensions of Nano-Sized Particles (Nanofluids), International Journal of Heat and Mass Transfer, 45 (2002), 4, pp. 855-863
- [9] Lee, S., et al., Measuring Thermal Conductivity of Fluids Containing Oxide Nanoparticles, Journal of Heat Transfer, 121 (1999), 2, pp. 280-289
- [10] Prasher, R., et al., Thermal Conductivity of Nanoscale Colloidal Solutions (Nanofluids), Physical Review Letters, 94 (2005), 2, 025901
- [11] Lin, B., et al., Direct Measurements of Constrained Brownian Motion of an Isolated Sphere between Two Walls, Physical Review E 62, (2000), 3, pp. 3909-3919
- [12] Benesch, T., et al., Brownian Motion in Confinement, Physical Review E, 68 (2003), 2, 021401
- [13] Iwashita, T., et al., Short-Time Motion of Brownian Particles in a Shear Flow, Physical Review E, 79 (2009), 3, 021401
- [14] Uma, B., et al., Nanoparticle Brownian Motion and Hydrodynamic Interactions in the Presence of Flow Fields, Physics of Fluids, 23 (2011), 7, 073602
- [15] Radiom, M., et al., Hydrodynamic Interactions of Two Nearly Touching Brownian Spheres in a Stiff Potential: Effect of Fluid Inertia, Physics of Fluids, 27 (2015), 2, 022002

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- [16] Mo, J., et al., Brownian Motion as a New Probe of Wettability, The Journal Of Chemical Physics, 146 (2017), 13, 134707
- [17] Cichocki, B., et al., Brownian Motion of a Particle with Arbitrary Shape, Physical Review E, 142 (2015), 21, 214902
- [18] Jahanshahi, S., et al., Brownian Motion of a Circle Swimmer in a Harmonic Trap, Physical Review E, 95 (2017), 2, 022606
- [19] Dessup, T., et al., Enhancement of Brownian Motion for a Chain of Particles in a Periodic Potential, Physical Review E, 97 (2018), 2, 022103
- [20] Landau, L. D., et al., Fluid Mechanics, Pergamon Press, London, UK, 1959
- [21] Aidun, C. K., et al., Lattice-Boltzmann Method for Complex Flows, Annual Review of Fluid Mechanics, 42 (2010), Jan., pp. 439-472
- [22] Nie, D., Numerical Investigation of a Capsule-Shaped Particle Settling in a Vertical Channel, *Thermal Science*, 16 (2012), 5, pp. 1419-1423
- [23] Xian, D. Q., et al., An Analytic Study on the Two-Temperature Model for Electron-Lattice Thermal Dynamic Process, *Thermal Science*, 21 (2017), 4, pp. 1777-1782
- [24] Ladd, A. J. C., Numerical Simulations of Particulate Suspensions via a Discretized Boltzmann Equation Part I. Theoretical Foundation, *Journal of Fluid Mechanics*, 271 (1994), July, pp. 285-309
- [25] Ladd, A. J. C., Numerical Simulations of Particulate Suspensions via a Discretized Boltzmann Equation, Part II. Numerical Results, *Journal of Fluid Mechanics*, 271 (1994), July, pp. 311-339
- [26] Nie, D., et al., A Fluctuating Lattice-Boltzmann Model for Direct Numerical Simulation of Particle Brownian Motion, Particuology, 7 (2009), 6, pp. 501-506
- [27] Alder, B. J., et al., Decay of the Velocity Autocorrelation Function, Physical Review A, 1 (1970), 1, pp. 18-21
- [28] Ailawadi, N. K., et al., Cooperative Phenomena and the Decay of the Angular Momentum Correlation Function at Long Times, *The Journal of Chemical Physics*, 54 (1971), 8, pp. 3569-3571

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