Preferential Brownian Motion Induced by a Fluid with Inhomogeneous Temperature

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Abstract. In the present work the fluctuating lattice Boltzmann method was used to numerically study the Brownian motion of particles in a fluid with inhomogeneous temperature. It has been shown that the Brownian particles are preferential to move into the cold fluid area due to small thermal fluctuations. In addition, the boundary between hot fluid and cold fluid prevents the particles going outside once they enter into the cold area. As a consequence, the Brownian particles can be captured or collected by the cold fluid area if the temperature of cold fluid is low enough.

1. Introduction
Brownian motion, also called Brownian movement, is the random motion of particles suspended in a fluid arising from those particles being struck by individual molecules of the fluid, which was named for the Scottish botanist Robert Brown. Brownian motion can be seen in many industrial applications. For instance, recent developments demonstrated that Brownian motion can help to measure the local viscoelastic response of soft materials [1] or the topography of a surrounding polymer network [2]. The trajectories of a Brownian particle can be used to characterize the mechanical properties of molecular motors [3]. In particular, experimental study [4, 5] showed that the nano-fluids exhibit enhanced thermal conductivity and convective heat transfer coefficients compared to those of base fluids, which is believed to be connected with the Brownian motion of nanoparticles [6].

In the past a variety of studies have been devoted to study the Brownian motion of particles in a viscous fluid because of its importance in industrial applications. Lin et al. [7] investigated the constrained Brownian motion of a sphere between two walls through an experimental work. The same problem was also studied by Benesch and Yioucumi [8] who used the method of reflection. Iwashita and Yamamoto [9] examined the effect of fluid inertia on the short-time motion of Brownian particles by using the direct numerical simulations. Recently, Radiom et al. [10] conducted an experiment to measure the hydrodynamic interactions between two Brownian spheres at low Reynolds numbers, to check the effect of fluid inertia. As is known, the Brownian motion is very sensitive to the temperature. Higher temperature leads to more-rapid Brownian motion. Brownian motion is isotropic if the temperature of fluid is homogeneous everywhere, which leads to a totally random movement of particles in the fluid. In other words, if a number of particles subject to Brownian motion are present in a given fluid and there is no preferred direction for the random oscillations, then over a period of time the particles will tend to be spread evenly throughout the medium. However, this may not be the truth if the temperature of fluid is inhomogeneous. For example, the Brownian motion may become preferential if there are hot fluid and cold fluid at the same time because the thermal fluctuations are determined by the temperature. However, as far as we know this issue has not been reported, which
motivates the present work. The fluctuating lattice Boltzmann method [11] is adopted in this work to study the preferential Brownian motion in a fluid with inhomogeneous temperature.

2. Numerical Method

The fluctuating lattice Boltzmann method is used to solve the fluid flow [11]. The discrete lattice Boltzmann equations are described by,

\[ f_i(x + e_i At + At) - f_i(x, t) = -\frac{1}{\tau} \left[ f_i(x, t) - f_i^{(eq)}(x, t) \right] + f_i^{(B)}(x, t) \]  

(1)

where \( f_i(x, t) \) is the distribution function on the \( i \)-direction discrete velocity \( e_i \), \( f_i^{(eq)}(x, t) \) is the equilibrium distribution function, \( At \) is the time step, \( f_i^{(B)}(x, t) \) is a stochastic term representing the thermal fluctuations, which is related to the fluctuating stress in the Navier-Stokes equations [11].

The macro-variables density \( \rho \) and momentum \( \rho u \) are obtained from,

\[ \rho = \sum_i f_i, \quad \rho u = \sum_i f_i e_i \]  

(2)

The equilibrium distribution function is chosen as,

\[ f_i^{(eq)}(x, t) = \rho \left[ 1 + \frac{e_i \cdot u}{c_s^2} + \frac{(e_i \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right] \]  

(3)

where \( c_s^2 = c^2/3 \) is the speed of sound.

As shown by Nie and Lin [11], the stochastic term is related to the fluctuating stress in the following way,

\[ \sigma_{ij}^{(B)} = -\tau \sum_i f_i^{(B)} e_{i\alpha} e_{ij} \]  

(4)

According to the fluctuation-dissipation theorem, \( \sigma_{ij}^{(B)} \) has the following property,

\[ \left\{ \sigma_{ij}^{(B)} \right\} = 0 \]  

\[ \left\{ \sigma_{ij}^{(B)}(x_1, t_1) \sigma_{kl}^{(B)}(x_2, t_2) \right\} = 2k_B T \mu \left( \delta_{il} \delta_{jk} + \delta_{ik} \delta_{jl} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \delta(x_1 - x_2) \delta(t_1 - t_2) \]  

(5)

where <> denotes averaging over an ensemble, \( k_B \) is the Boltzmann constant, \( T \) is the temperature of fluid, \( \mu \) is the dynamic viscosity of the fluid. The fluctuating stress is sampled from a Gaussian distribution with zero mean and a given variance of \( 2k_B T \mu \).

In this work we assume the stochastic term \( f_i^{(B)}(x, t) \) to be the following form to make sure of the conservation of mass and momentum [11],

\[ f_0^{(B)} = 0 \]

\[ f_1^{(B)} = f_3^{(B)} = \frac{1}{2\tau} \sigma_{xy}^{(B)} \]

\[ f_2^{(B)} = f_4^{(B)} = \frac{1}{2\tau} \sigma_{xx}^{(B)} \]

\[ f_5^{(B)} = f_7^{(B)} = \frac{1}{4\tau} \left( \sigma_{xx}^{(B)} + \sigma_{yy}^{(B)} + \sigma_{xy}^{(B)} \right) \]

\[ f_6^{(B)} = f_8^{(B)} = \frac{1}{4\tau} \left( \sigma_{xx}^{(B)} + \sigma_{yy}^{(B)} - \sigma_{xy}^{(B)} \right) \]  

(6)

3. Validation

The Brownian motion of 81 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 \( 240 \times 240 \). 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 fluid \( \nu = (2\tau - 1)/6 = 0.05 \). The radius of particle is \( a = 3.5 \). The
solid/fluid density ratio is fixed at $\rho_s/\rho = 11$ in the simulations. In order to determine the magnitude of the fluid fluctuation, the temperature of fluid is chosen as $k_B T = 10^{-4}$.

The instantaneous fluctuations of fluid pressure at different times are shown in Fig. 1, along with the Brownian particles, which clearly illustrate the thermal fluctuations. This is the origin of the Brownian motion of particles, resulting from the essence of the present fluctuating lattice Boltzmann method, 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.

The long time tails can be used to validate the effectiveness of numerical method. Fig. 2 shows the translational and rotational velocity autocorrelation functions (VACFs) of particles. In the figure $U$ and $V$ refer to the translational velocity, and $\Omega$ refers to the rotational velocity. All the results are normalized by their initial values, i.e. the values at $t = 0$. According to the theoretical predictions, the translational and rotational VACFs of particles undergoing Brownian motion have power-law decays over long times that are $t^{-1}$ and $t^{-2}$, respectively. As shown in Fig. 2, the similar long time tails are observed for the particles in the present simulations, which is consistent with the theoretical prediction.

4. Numerical Results

First of all, the Brownian motion of a circular particle in a fluid with inhomogeneous temperature is numerically investigated. The particle is freely moving in the domain of $L \times L$, which is filled with the hot fluid with temperature $T_h$. There is a circular area with radius $R$ inside which the fluid is cold. The
temperature is denoted as $T_c$. For simplicity the no-slip boundary conditions are imposed on all four fixed walls of the domain. In all simulations, the parameters are fixed at $a = 3.5$, $R_a = 3.5 a$, $T_h = 1.0 \times 10^{-3}$ and $\rho_s / \rho = 11$. The particle is initially placed in the center of the domain.

Fig. 3 shows the instantaneous flow (the magnitude of fluid velocity $|u|$ normalized by $v/a$) of particle Brownian motion at different times. The computational domain is $64 \times 64$. Two kinds of cold temperature are taken into account, i.e. $T_c = 1.0 \times 10^{-3}$ (top) and $5.0 \times 10^{-5}$ (bottom). For the results of $T_c = 1.0 \times 10^{-3}$, 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 the other results. By displaying the RMS of fluid velocity a cold temperature zone is observed in the central area, as can be seen in Fig. 3. For the case of $T_c = 1.0 \times 10^{-3}$, the particle is randomly moving in the whole domain. However, the particle will exhibit preferential Brownian motion when there is cold fluid. In other words, the particle prefers to move into cold fluid area. 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 $T_c = 5.0 \times 10^{-5}$. This makes it possible that the Brownian can be captured by the cold temperature area somewhere in the fluid.

![Figure 3](image)

**Figure 3.** Instantaneous flow (the magnitude of fluid velocity $|u|$ normalized by $v/a$) of Brownian motion at different times: (a) $t=1 \times 10^4$, (b) $t=1 \times 10^5$, (c) $t=4 \times 10^5$, (d) $t=1 \times 10^6$. The values of $T_c$ are $1 \times 10^{-3}$ (top) and $5 \times 10^{-5}$ (bottom).

In what follows another two cases are presented to further illustrate the influence of fluid temperature. The first case is depicted in Fig. 4, showing the instantaneous flow of Brownian motion of 16 particles at different times. The computational domain is $240 \times 240$. The left half of domain is set to be cold area with temperature $T_c = 5 \times 10^{-5}$. At the beginning of simulations, the particles are placed homogeneously over the computational domain, as one can see in Fig. 4(a). The cold fluid results in very small thermal fluctuations in the left part of domain, as a consequence, most of particles quickly go into the cold area and do not leave, which can be seen in Fig. 4. The second case is illustrated in Fig. 5, which shows the preferential Brownian motion of 36 particles in an inhomogeneous fluid. For this case the cold area is located in the center of domain, instead. Other parameters are the same to those used in the case of Fig. 3. Generally speaking, similar behavior is observed from Fig. 5. The cold area captures almost all particles when they are randomly moving in the fluid. However, it will take 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.
In the final, it should be stated that the viscosity is kept constant for every single simulation in this work. However, it is believed that there exist some fluids whose viscosities are not sensitive to the temperature. Therefore, the conclusion of this work still stands for these fluids.

5. Summary
In this work the fluctuating-lattice Boltzmann method was adopted to numerically investigate the preferential Brownian motion of particles in a fluid with inhomogeneous temperature. Results show that the particles are preferential to randomly move in 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. In other words, the cold fluid can capture or collect the Brownian particles.

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