Focusing of Brownian Particles in a Fluid Induced by the Temperature Difference

Yuxiang Ying, Kaixuan Zheng and Deming Nie

Institute of Fluid Mechanics, China Jiliang University, Hangzhou 310018, China
Email: nieinhz@cjlu.edu.cn

Abstract. In this work the Brownian motion of particles in a two-dimensional channel was numerically studied through a fluctuating-lattice Boltzmann method. The effects of the fluid temperature difference on the biased Brownian motion of particles were examined. It is shown that the particles are likely to move towards and stay at the low temperature zone. More importantly, the focusing of Brownian particles may be realized if the temperature difference is large enough. This paper also provides a quantitative analysis on this issue.

Keywords. Brownian motion, focusing, lattice Boltzmann method.

1. Introduction

Brownian motion, the random movement of submicro/nano particles suspended in a liquid or gas, is caused by collisions between these particles and the molecules of the liquid or gas. Brownian motion is very common in nature as well as in many engineering fields. The nanofluid may be one of the most famous examples. Experimental study [1, 2] demonstrated that the nanofluids exhibit enhanced thermal conductivity and convective heat transfer ability compared to those of base fluids, which is believed to be connected with the Brownian motion of nanoparticles (e.g., nano metals or metal oxides) [3].

Due to its significance both in engineering and academic fields, much effort has been dedicated to the study of particle Brownian motion. For example, the Brownian motion constrained between two walls was experimentally investigated by Lin et al. [4]. Similarly, Benesch and Yiacoumi [5] studied the wall effects through a numerical method. In particular, the short-time characteristics of the Brownian motion were checked by Iwashita and Yamamoto [6] who performed direct numerical simulations of a sphere driven by thermal fluctuations of a fluid. The hydrodynamic interactions between two Brownian particles were experimentally examined by Radium et al. [7]. Recently, the motion of active Brownian particles (also known as microswimmer) has received much attention. In comparison with the passive Brownian particles, the microswimmers propel themselves with directed motion and exhibit out-of-equilibrium nature. Volpe et al. [8] proposed a mathematical model to simulate the motion of active Brownian particles in homogeneous and complex environments which is based on a set of stochastic differential equations. Ouyang et al. [9] presented a numerical study on the motion of microswimmers near a wall using an immersed boundary – lattice Boltzmann method. Three types of microswimmer (i.e., pusher, neutral swimmer and puller) were taken into their study. Reinken et al. [10] developed a fourth-order continuum theory to account for the collective behaviours of a large number of microswimmers in a Newtonian fluid.

It is known that the fluid temperature is a key factor which largely determines the intensity of the Brownian motion of particles. In other words, the Brownian particles move randomly at a higher speed...
in a hot fluid than in a cold fluid because the flow fluctuations are directly linked to the fluid temperature. If the fluid temperature is the same everywhere, which is the common case, each Brownian particle moves in any direction with the same possibility. This results in the classical Brownian diffusion. However, things may be quite different if there is a temperature difference in the fluid. Our previous study [11] showed that the Brownian motion may become biased when the fluid temperature is not homogeneous. That is, most of Brownian particles were observed to go into the cold area from the hot area. This trend is getting more significant as the temperature difference is larger [11]. As a first step towards the study on the biased Brownian motion, it was assumed that there is no transition region from the hot region to cold region in our previous work [11]. In other words, a sharp interface was used to separate the cold fluid and hot fluid, which does not exist in the real world. To improve the energy equations along with a parameter of heat diffusion coefficient were introduced to solve the fluid temperature in this work. Similarly, the fluctuating lattice Boltzmann method [12] was employed in this work to study the effects of fluid temperature difference on the focusing of Brownian particles.

2. Method
The fluctuating-lattice Boltzmann method (FLBM) [12] was implemented to solved the motion of fluid. A brief description of the FLBM is provided here. The lattice Boltzmann equations are given by,

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

where \( f_i(x, t) \) is the distribution function corresponding to the \( i \)-th discrete velocity \( e_i \); \( f_i^{(eq)}(x, t) \) is the equilibrium distribution function, \( \Delta t \) is the time step and \( \tau \) is the relaxation time. In particular, a stochastic term, i.e. \( f_i^{(b)}(x, t) \), is introduced to represent the thermal fluctuations of fluid, which is related to the fluctuating stress in the Navier-Stokes equations [12].

The fluid density \( \rho \) and velocity \( u \) are calculated through the following formulations,

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

The D2Q9 lattice model, which is very popular for two-dimensional lattice Boltzmann computations, can be formulated by its velocity vectors as follows,

\[ e_i = \begin{cases} (0,0), & \text{for } i = 0, \\ (\pm1,0)c, (0,\pm1)c, & \text{for } i = 1 \text{ to } 4, \\ (\pm1,\pm1)c, & \text{for } i = 5 \text{ to } 8, \end{cases} \]

where \( c = \Delta x / \Delta t \) and \( \Delta x \) is the lattice spacing. The equilibrium distribution functions are chosen as,

\[ f_i^{(eq)}(x, t) = w_i \rho \left[ 1 + \frac{3e_i \cdot u}{c^2} + \frac{4.5(e_i \cdot u)^2}{c^4} - \frac{1.5u \cdot u}{c^2} \right] \]

where the weights are assumed to be \( w_0 = 4/9, w_{1,4} = 1/9 \) and \( w_{5,8} = 1/36 \).

As shown in [12], the relationship between the stochastic term and the fluctuating stress is formulated as,

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

According to the fluctuation-dissipation theorem, the following equations need to be satisfied [12],
\[ \left< \sigma^{(B)}_{\alpha\beta} \right> = 0 \]
\[ \left< \sigma^{(B)}_{\alpha\beta} (x,t) \sigma^{(B)}_{\gamma\delta} (x',t') \right> = 2 \mu T \left( \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma} - \frac{2}{3} \delta_{\alpha\beta} \delta_{\gamma\delta} \right) \delta_{xx} \delta_{yy} \] (6)

where \( \left< \right> \) represents averaging over an ensemble, \( k_B \) is the Boltzmann constant, \( T \) and \( \mu \) are the fluid temperature and dynamic viscosity, respectively. Note that each member of the fluctuating stress tensor is sampled from a Gaussian distribution with zero mean and a given variance of \( 2k_B T \mu \).

By using a Chapman-Enskog expansion, the Navier-Stokes equations can be recovered from the lattice Boltzmann equations [12].

\[ \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0 \] (7a)
\[ \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -\partial_\alpha p + \nu \partial_\beta \left[ \partial_\alpha (\rho u_\beta) + \partial_\beta (\rho u_\alpha) \right] + \partial_\beta \sigma^{(B)}_{\alpha\beta} \] (7b)

The kinematic viscosity of fluid is determined through \( n = \nu^2 \Delta t \). According to equation (5), the stochastic term was assumed to have the following forms which guarantee the conservation of mass and momentum [11],

\[ f_0^{(B)} = 0 \]
\[ f_1^{(B)} = f_3^{(B)} = \frac{1}{2\tau} \sigma^{(B)}_{yy} \]
\[ f_2^{(B)} = f_4^{(B)} = \frac{1}{2\tau} \sigma^{(B)}_{xx} \]
\[ f_5^{(B)} = f_7^{(B)} = -\frac{1}{4\tau} \left[ \sigma^{(B)}_{xx} + \sigma^{(B)}_{yy} + \sigma^{(B)}_{xy} \right] \]
\[ f_6^{(B)} = f_8^{(B)} = -\frac{1}{4\tau} \left[ \sigma^{(B)}_{xx} + \sigma^{(B)}_{yy} - \sigma^{(B)}_{xy} \right] \] (8)

In addition, the bounce-back scheme proposed by Ladd [13] was applied to deal with the curved surfaces of solid particles. The hydrodynamic force and torque of particles were computed through the momentum-exchange method. Then the Brownian motion of particles can be updated by solving the Newton’s equations.

3. Problems
This work aims to present a numerical study on the focusing of Brownian particles caused by the fluid temperature difference. As illustrated in figure 1, multiple particles with density \( \rho_p \) and diameter \( d \), confined in a two-dimensional channel with length \( L \) and height \( H \), undergo Brownian motion due to the random collisions of fluid molecules. The density and viscosity of fluid are denoted as \( \rho_f \) and \( \nu \), respectively. It is assumed that the channel walls have a higher temperature \( (T_w) \) than that of the fluid \( (T_f) \), i.e., \( T_w \geq T_f \). The temperature distribution is then determined through solving the energy equations for which another set of lattice Boltzmann equations were adopted [14]. For more details, readers are referred to [14]. It should be noted here that the fluid temperature difference depends strongly on the heat diffusion coefficient of the fluid (\( \alpha \)).
For this work some parameters are fixed as follows: $\rho_f = 1$, $T_f = 10^{-4}$, $\nu = 1/100$, $\alpha = 1/600$, $\rho_p = 10$, $d = 13$. The channel height is fixed at $H = 10d$ and its length $L = 4H$. Note that all parameters are all in lattice units. A dimensionless parameter, i.e., $\lambda = T_w/T_f$, was introduced to represent the temperature ratio of the channel walls to the fluid.

In addition, no-slip boundary conditions were imposed on both walls of the channel, as shown in figure 1. Both lateral sides of the channel were assumed to be periodic, which indicates that one particle comes into the channel from the left side once it leaves from the right side, and vice versa.

4. Results

For the sake of saving space, the validation was not included in this paper since the effectivity of the fluctuating–lattice Boltzmann method has been examined in our previous work [11, 12]. For all cases in this work, an array of particles with 5 rows and 20 columns (i.e., 20×5) were initially placed in the channel with equal interparticle distance. It is obvious that the number of the particles is 100.

Figure 2 shows the instantaneous flow fluctuations at different times for $\lambda = 1$, which corresponds to the case of $T_w = T_f$. The fluctuations are illustrated by showing the normalized magnitude of the fluid velocity, i.e., $|\mathbf{u}|/U_c$. The reference velocity, i.e., $U_c$, is defined as $U_c = (k_B T/M)^{1/2}$. Note that $M$ is the mass of a particle. As shown in figure 2, the particles undergo random walks in the channel since there is no temperature difference. As a result, a random but homogeneous distribution of the particles is always seen due to the hydrodynamic interactions and collisions between them [figure 2(b, c)]. This is the classical Brownian diffusion.

The situation becomes different when the channel walls are heated. That is, the temperature of the walls is higher than that of the fluid. Figure 3 shows the corresponding results for $\lambda = 5$, i.e., $T_w = 5T_f$. It is seen that the flow fluctuations adjacent to the walls are much stronger than those at the central area of the channel, reflecting the temperature difference in the fluid. It appears that most of the
particles at the high temperature zone eventually move into the central area of the channel, as shown in figure 3. The particles exhibit a pattern of biased Brownian motion, which differs from the classical Brownian diffusion (figure 2). The mechanism behind this can be explained as follows. A particle undergoing Brownian motion experiences a larger random force when it is surrounded by a hot fluid than by a cold fluid. Therefore, the particles may be pushed back by the hot fluid when they are trying to move into the high temperature zone from the low temperature zone. If the temperature difference is large enough, the interface between the hot fluid and cold fluid may act as a barrier which prevents the particles from crossing. This is further illustrated by figure 4(a, b), which shows the final state of the particle distribution for $\lambda = 10$ and $\lambda = 15$, respectively.

![Figure 3. The same as figure 2 except $\lambda = 5$ (i.e., $T_w = 5T_f$).](image)

It is seen from figure 4 that most of the particles are focusing at the central area of the channel due to very strong flow fluctuations near the walls. The larger the temperature difference is, the more significant the focusing of particles is [figure 3(c) and figure 4(a, b)]. This suggests that the biased Brownian motion induced by a temperature difference can be used to drive small particles (sub-micro and nano particles) to a certain region, e.g., the central area of a channel/tube or the corners of a container.

![Figure 4. Final state of the particle distribution in the channel for (a) $\lambda = 10$ and (b) $\lambda = 15$, respectively.](image)

To provide a quantitative analysis on the particle focusing, a dimensionless parameter was introduced,
\[ Y(t) = \frac{2 \sum_{i=1}^{N} \sqrt{y_i^2(t)}}{NH} \]  
(9)

where \( y_i(t) \) is the vertical position of the \( i \)-th particle and \( N \) denotes the number of the particles. This definition indicates that \( Y(t) \) represents the averaged distance between all particles and the channel axis (see also figure 1). The smaller the value of \( Y(t) \) is, the more prominent the focusing is. Figure 5 shows the time history of \( Y(t) \) for all values of \( \lambda \) considered. It is seen that \( Y(t) \sim 0.5 \) for \( \lambda = 1 \) which corresponds to the case of homogeneous fluid temperature. This is in accord with the nature of the classical Brownian diffusion. However, for \( \lambda \geq 5 \) the value of \( Y(t) \) is seen to decrease sharply with time at \( t > 10^3 \), suggesting that the particles are driven to move towards the central area of the channel. It is obvious that \( Y(t) \) reaches a smaller minimum value for a larger \( \lambda \), which is consistent with the observation made in figure 3 and figure 4.

**Figure 5.** Time history of the averaged distance between the particles and the channel axis \([Y(t)]\) for different temperature ratios \((\lambda)\).

**5. Conclusion**
A two-dimensional fluctuating lattice Boltzmann method was used to simulate the Brownian motion of particles in a fluid which is confined in a channel. Much attention was paid to a pattern of biased Brownian motion induced by the fluid temperature difference. Results reveal that the Brownian particles are likely to move towards and eventually stay at the low temperature zones of the fluid. This may lead to the focusing of Brownian particles if the temperature difference is large enough. The effects of the fluid viscosity, heat diffusion coefficient and the particle inertia will be further examined in the future work.

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