Influence of walls on the migration of non-Brownian spherical particles in creeping flow: a lattice Boltzmann study

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The influence of walls on binary encounters of spherical particles under creeping flow is studied by means of the lattice Boltzmann method. Depending on the initial particle displacement different behaviours can be observed, including the ‘swapping’ trajectories. The domain of the swapping trajectories is identified for interacting spheres with the same diameter; some preliminary results are given for the case of two spheres with different diameters. Finally, the influence of particle swapping on the dynamics of monodisperse suspensions is also described.

Keywords: shear flow; particle interactions; lattice Boltzmann method

1. Introduction

Particle distribution in non-Brownian suspensions is greatly influenced by hydrodynamic cross-streamline migration induced by particle encounters. To achieve a complete understanding of such phenomena, it is worth starting with the simplest possible configuration, consisting of two spherical particles interacting in a shear flow. At the creeping-flow regime, the Stokes equation holds: according to this equation, in an unbounded flow, the faster (trailing) particle overtakes the slower (leading) one and both particles return to their original transverse position once the encounter terminates [1]. That means at least three particles are required for cross-streamline diffusion in the absence of non-hydrodynamic forces breaking the symmetry of the flow.

The presence of walls can significantly change this situation: as shown in Zurita-Gotor et al. [2], if the flow is bounded by walls and the channel height is compatible with the particle diameter, a new class of trajectories can be observed in which the trailing particle does not overtake the leading one; rather, the transverse component of the relative particle velocity changes sign, leading to an exchange of the vertical positions of the particles. The occurrence of these swapping trajectories depends on the initial particle displacement: in Zurita-Gotor et al. [2], the domain of the swapping trajectories was identified for the case of spheres with the same diameter. A Cartesian representation

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algorithm [3] was used in their study. The influence of walls and the consequent occurrence of swapping trajectories were found to explain the unexpectedly high self-diffusion coefficient measured in the experiments of Zarraga & Leighton [4].

In this study, the lattice Boltzmann (LB) method [5] is instead adopted. The LB equation derives from a convenient discretization of the Boltzmann equation on a finite set of $b$ speeds and describes the evolution of $b$ probability distributions $f_i$ of fictitious particle populations owing to streaming and collisions. The collision is completely local and relaxes each $f_i$ to its equilibrium value $f_i^{eq}$, which depends on local macroscopic density and speed, while the streaming step simply consists of shifting the distributions to the next-neighbour node. The incompressible Navier–Stokes equation is recovered in the limit of low Mach number, provided the lattice and the $f_i^{eq}$ are carefully chosen. Density, momentum and energy are obtained as discrete momenta of the $f_i^{eq}$, while the pressure is given by an equation of state and the kinematic viscosity is directly controlled by the collision frequency [5]. More details concerning the models adopted in this study can be found in Ladd [6] and Nguyen & Ladd [7]. The rest of the paper is organized as follows: §2 describes the geometry of the studied cases, while §3 illustrates the results for the cases of the same and different radii and §4 concludes the paper.

2. System description

The configuration of the system considered in this study is shown in figure 1: the dispersed phase consists of two non-Brownian spherical particles, identified, respectively, as the faster, or ‘trailing’ (particle 1), and the slower, or ‘leading’ (particle 2), particle, characterized by diameters $d_1$ and $d_2$. The characteristic length of the problem $d$ is always assumed to be the diameter of the biggest particle. They move in a Couette flow characterized by a shear rate $\alpha$ in a channel bounded by walls on $x$–$z$ planes separated by distance $H$. The continuous phase has the same density as the particle and kinematic viscosity $\nu$. We studied the relative motion of particle 2 with respect to particle 1; thus, we introduce the relative coordinates $\Delta r = (\Delta x, \Delta y, \Delta z)$. The unperturbed speed at a given height $y$ is given by $U = ay\epsilon y$, while the maximum speed on the top wall is $U_0$. The other boundaries are periodic. The flow is characterized by the shear Reynolds number $Re_\alpha = ((d/2)^2\alpha)/\mu$, which is held equal to 0.001 in this study. The particle diameter is 20 in lattice units, unless otherwise specified. Three configurations have been considered in this study: first, the case in which both particles have the same diameter, $d_1 = d_2$, then, the case in which the leading particle has twice the diameter of the trailing one, $d_2 = 2d_1$, and, finally, the case $d_1 = 2d_2$.

All the different observable trajectories are shown in figure 2. In an unbounded shear flow, the relative $\Delta y$ increases while the leading particle is approached by the trailing one until a maximum is reached at $\Delta z = 0$; the particles then return to their initial transverse positions. For bounded flow, the outcome depends on the initial displacement $\Delta y_0$. For sufficiently large $\Delta y_0$, the evolution is similar to the unbounded case, except for a minimum reached before $\Delta z = 0$; decreasing $\Delta y_0$ can lead to completely different trajectories, characterized by a change in sign of $\Delta y$: the leading particle will never be reached by the trailing one, until there is a

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swap of the transverse coordinates. In Zurita-Gotor et al. [2], it was shown that the swapping trajectories depend on the walls, which scatter the perturbation flow $\delta u$ induced by a moving particle, inducing motion towards the channel centre of the second particle.

3. Results

As the first test, we report in figure 3 the trend with time of the relative interparticle gap, defined as $\epsilon = |\Delta r|/d - 1$ for the different initial transverse offsets $\Delta y_0$ reported in Zurita-Gotor et al. [2]. Here $H/d = 5$. The different configurations, as well as the observed outcomes, are reported in table 1, which

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Figure 3. Interparticle relative distance ($\epsilon$) with time for the case of particles with the same diameter. Swapping trajectories are identified by the heavy lines.

Table 1. Summary of the different configurations tested in this study and in Zurita-Gotor et al. [2]. A tick mark (✓) indicates that the $\Delta y_0$ of that configuration will lead to a swapping trajectory, while a cross symbol (×) indicates a non-swapping case.

<table>
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<tr>
<th>configuration</th>
<th>$\Delta y_0 / d$</th>
<th>$d_1 = d_2$ [2]</th>
<th>$d_1 = d_2$ (LB)</th>
<th>$d_1 = 2d_2$ (LB)</th>
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</tr>
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shows perfect agreement between this study and that of Zurita-Gotor et al. [2]. Some of these trajectories are shown in figure 3, from which it is possible to observe how the occurrence of swapping prevents particle contact. In fact for swapping trajectories $\epsilon = O(1)$, while the gap for the non-swapping case can decrease down to $\epsilon = 10^{-3}$. Figure 4 shows the trend of the relative gap for the cases $d_2 = 2d_1$ (figure 4a) and $d_1 = 2d_2$ (figure 4b). The behaviour is similar to the previous case, with the only difference being that the minimum distance for the non-swapping cases is higher.

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The next test consists in determining how the offset in the flow direction \( \Delta z \) influences the occurrence of swapping trajectories. Given the configuration depicted in figure 1, it is clear that swapping occurs only when particles cross the plane \( \Delta y = 0 \) with \( \Delta U_y > 0 \). Therefore, we placed two particles at the same \( y \) and we observed the trajectories corresponding to different \( \Delta z \). The observations for particles at different heights over the lower wall in a channel with \( H/d = 5 \) are collected in figure 5 for particles with same diameter. From figure 5, it is possible to observe that the critical distance \( \Delta \rho_{\text{crit}} = \Delta x_{\text{crit}} e_x + \Delta z_{\text{crit}} e_z \) does not depend

\[ \Delta U_y / (d\alpha) \]
Figure 6. Normalized radius $\Delta r_{\text{crit}}$ of the circle of zeros of $\Delta U_y$ versus the channel width $H$ for a pair of particles in the midplane. (a) Particles with same diameter. Dashed-dotted line with squares, Zurita-Gotor et al. [2]; solid line with triangles, LBM; dashed line, asymptotic. (b) Cases of particles with different diameters. Dashed-dotted line with circles, LBM $d_1 = 2 \times d_2$; dashed line with diamonds, LBM $d_2 = 2 \times d_1$; dashed line, asymptotic.

on the orientation of $\Delta r$ in the $\Delta y = 0$ plane [2] and limits the domain of the swapping trajectories: if $|\Delta r| < \Delta r_{\text{crit}}$ when $\Delta y = 0$ no swapping will occur. In all cases, the peak is reached when the couple of particles is close to the lower wall. Figure 6a shows how close our simulations are to the asymptotic scaling as well as to the numerical results proposed in Zurita-Gotor et al. [2]. The same scaling is reported as the reference for the cases of particles with different diameters: substantially the behaviour is very similar, but the critical distance is reduced at every $H$ with respect to the case of particles with the same diameter.

In order to evaluate the influence of the offset in the vorticity direction, a series of tests were performed again at different channel heights. For each $H/d$, a couple of particles symmetrical with respect to the axis defined by the intersection of planes $x = (x_1 + x_2)/2$ and $y = H/2$ is considered: while $\Delta x$ is varied, the corresponding initial $\Delta z$ is the one making $\Delta U_y = 0$ for that configuration [2]. As can be inferred from figure 7, there is substantial agreement with the results reported in Zurita-Gotor et al. [2] for the case $d_1 = d_2$.

In order to evaluate the influence that swapping trajectories exerts on a non-Brownian dilute particle suspension, we have considered the Couette flow in a parallel-wall channel with $H/d = 5$ of a mixture of two species of particles with the same diameter. Particles of species 1 (indicated by diamonds in figure 8a) were initially placed in the region $y < H/2$, while particles of species 2 (indicated by squares in figure 8a) were initially placed in the $y > H/2$ region. The grid in this case is given by $100 \times 100 \times 600$ lattice nodes. A total of 1100 particles whose diameter is 10 lattice units, resulting in a volume fraction of $\phi = 0.1$, were placed in this domain. Ten simulations were performed; the results were averaged in order to reduce statistical fluctuations. The initial and final conditions related to one of these runs can be observed in figure 8a, b, respectively, from which a substantial amount of mixing, which is entirely owing to the swapping mechanism because of the low $\phi$, can be appreciated.
LB study of particle encounters

Figure 7. Initial displacements in plane $x-y$ corresponding to swapping trajectories for particles symmetrical to the midplane. The curves are calculated at different $H/d$ for $d_1 = d_2$ and compared with corresponding results given in Zurita-Gotor et al. [2]. Swapping occurs in the regions below each curve. Squares, $H/d = 1.75$ LB; solid line, $H/d = 1.75$ [2]; triangles, $H/d = 20$ LB; dashed line, $H/d = 20$ [2]; inverted triangle, $H/d = 3.19$ LB; dashed-dotted line, $H/d = 3.19$ [2]; diamonds, $H/d = 40$ LB; long dashed line, $H/d = 40$ [2]; circles, $H/d = 5.36$ LB; dash with double-dotted line, $H/d = 5.36$ [2].

Figure 8. (a) Initial and (b) final distribution of particles of species 1 (squares) and species 2 (diamonds).

To make a quantitative analysis, we computed the dimensionless contribution $D_{swa}^{\text{p}}$ given by the swapping trajectories to the self-diffusivity coefficient [2],

$$D_{swa}^{\text{p}} = 6\pi^{-1}\alpha \int_{-\infty}^{\infty} \Delta y_{\text{smax}}^2 \, d\Delta x.$$  \hspace{1cm} (3.1)
In equation (3.1), $\Delta y_{\text{max}}^4 = \Delta y_{\text{max}}^4(\Delta x)$ is the limit of the swapping trajectory domain shown in figure 7. From this equation, it is clear that $D_{\text{swap}}$ depends on the position $y$ of the $\Delta y = 0$ plane for each couple of particles under consideration. An evaluation of equation (3.1) for different values of $H/d$ is reported in figure 9, which shows a satisfactory comparison with the analogous results in Zurita-Gotor et al. [2].

4. Conclusion

The influence exerted by planar walls on the interactions among non-Brownian spherical particles in shear flow was investigated using the LB method. This mesoscopic approach allows easy modelling of moving objects and of their interactions with the suspending fluid. All the different kinds of trajectories predicted in Zurita-Gotor et al. [2] for particles with the same diameter were observed, reconstructing the range of initial particle displacement leading to particle swapping. The results match those reported in Zurita-Gotor et al. [2]. In addition, some preliminary extension to the case of particles with different diameters was reported. The latter needs definitively to be extended by examining the contribution of swapping in bidisperse suspensions, as well as either the presence of rough walls or the occurrence of the so-called electroviscous effect that may influence the domain of the swapping trajectories. All these points will be the subject of future studies.

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References


