Sedimentation of two unequal spheres in a square tube at low Reynolds numbers

Geng Guan, Yuxiang Ying, Deming Nie*
Institute of Fluid Mechanics, China Jiliang University, Hangzhou, China

*Corresponding author: nieinhz@cjlu.edu.cn

Abstract. The settling behaviors of two unequal spheres in a square tube at low Reynolds numbers were numerically studied through a three-dimensional lattice Boltzmann method (LBM). Due to the hydrodynamic interaction, a periodic state or a steady state is achieved according to the density ratio between the spheres. In addition, it is seen that the spheres form a staggered stable configuration at the steady state, for which both spheres rotate in the same manner. The effects of the Reynolds number were also examined.

Keywords: sedimentation, unequal spheres, interaction, lattice Boltzmann method

1. Introduction
The motion of solid particles in a fluid driven by the gravity is very common in nature as well as in engineering applications. As is known, the particles may interact with each other when they are falling or rising in the fluid. The situation could be more complicated as the fluid inertia gets stronger. For instance, the vortex-shedding may occur due to the boundary layer separation at high fluid inertia, which results in the oscillations of particles. In addition, a particle may attract other particles because of the strong wake effects. The classical drafting, kissing and tumbling (DKT) motion is one of the most famous examples. The DKT was firstly reported by Fortes et al. [1], who conducted an experimental study on the sedimentation and interaction of two spheres. Feng et al. [2] reproduced the same phenomenon for two circular cylinders through direct numerical simulations. Correspondingly, it is possible that a large number of particles aggregate and settle as a cluster in the fluid because of the wake effects. The cluster may greatly influence the flow features as well as the motion and dynamics of particles. It was revealed [3] that the settling velocity of particles could be significantly enhanced by the clustering of particles. The mechanism is not well understood. However, it was believed that the interaction of particles plays a key role in the clustering of particles and the resulting enhanced velocity. In fact, numerical studies showed that the motion of particles may exhibit a rich set of dynamical features even at low but finite fluid inertia. For example, Aidun & Ding [4] studied the sedimentation and interaction of two circular particles under gravity in a 4d (d is the diameter of particle) channel using the lattice Boltzmann method. According to their work, a variety of patterns of particle motion (i.e., the periodic state, chaotic state, and periodic-doubling bifurcation) can be observed at low Reynolds numbers. By extending the range of Reynolds number, Verjus et al. [5] reported new features of the same sedimentation system and established a link between the terminal Reynolds number and the non-dimensional driving force using a global diagram that illustrates the dynamic features of particles in a
Recently, Nie & Lin studied the interaction of two particles with different densities in gravity-driven flows in both two dimensions [6] and three dimensions [7]. The two-dimensional analysis [6] shows that there exists a discontinuous change in the settling velocity of particles as well as in the time period of particle oscillations at a certain density difference between particles. The discontinuity in the latter was found to have relation with the change in the rotation direction of heavy particle [6]. However, no discontinuity was found in either of the period and velocity of particles for the three-dimensional analysis [7].

When the Reynolds number is low the spherical particles may move to the diagonal (or inverse diagonal) plane of a square tube which are released from rest in the center-line plane.

There are extensive studies on the motion and interaction of particles in two dimensions. By the contrast, limited attention has been paid to the motion of spheres at finite or moderate fluid inertia due to huge memory requirements and high computational costs. Much effort was devoted to the Stokes flow for which the fluid inertia is neglected. As stated above, the wake effects, resulting from the fluid inertia, could add complexity to the dynamical features of a fluid-particle system. To provide valuable insights into this issue, it is necessary to perform three-dimensional studies on the motion of particles at non-zero Reynolds numbers. On the other hand, our previous work [6, 7] considered the case of flows containing particles with the same size but different densities. On this basis, the more general case of particles having different sizes and different densities were taken into account in this study. The focus is on the interaction of two unequal spheres in gravity-driven flows at low Reynolds numbers.

2. Method

The motion of fluid was solved through a three-dimensional lattice Boltzmann method in this work. The discrete lattice Boltzmann equations of a single-relaxation-time model are expressed as [8],

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

(1)

Where \( f_i(x, t) \) is the distribution function for the microscopic velocity \( e_i \), \( f_i^{(eq)}(x, t) \) is the corresponding equilibrium distribution function, \( \Delta t \) is the time step of the simulation, \( \tau \) is the relaxation time associated with the fluid viscosity, and \( w_i \) are weights related to the lattice model. The fluid density \( \rho \) and velocity \( u \) are obtained through the following formulations,

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

(2)

For the D3Q19 (i.e. nineteen velocities in three dimensions) lattice model used here, the discrete velocity vectors are [8],

\[ e_i = \begin{cases} (0,0,0)c & i = 0 \\ (\pm1,0,0)c, (0,\pm1,0)c, (0,0,\pm1)c & i = 1 \sim 6 \\ (\pm1,\pm1,0)c, (\pm1,0,\pm1)c, (0,\pm1,\pm1)c & i = 7 \sim 18 \end{cases} \]

(3)

Where \( c = \Delta x/\Delta t \), and \( \Delta x \) is the lattice spacing. The speed of sound is determined through \( c_s = c/\sqrt{3} \).

Following Qian [8], the equilibrium distribution function is chosen as,

\[ f_i^{(0)}(x, t) = w_i \rho \left[ 1 + \frac{3 e_i \cdot u}{c^2} + \frac{9 (e_i \cdot u)^2}{2c^4} - \frac{3 u^2}{2c^2} \right] \]

(4)

Where the weights are set to be \( w_0 = 1/3, w_{1 \sim 6} = 1/18 \) and \( w_{7 \sim 18} = 1/36 \).
By performing a Chapman–Enskog expansion, the macroscopic mass and momentum equations in the low-Mach-number limit can be recovered:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

(5)

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u}
\]

(6)

In this method, the fluid viscosity is computed using \( \nu = c_s^2 \Delta t (\tau - 0.5) \). For simplicity, both the lattice spacing and time step is set to be 1 in the simulations, i.e. \( \Delta x = \Delta t = 1 \), unless otherwise stated.

In LBM the boundary conditions need to be handled in a special way. For example, the simple bounce-back scheme was usually adopted to satisfy the non-slip conditions of solid surfaces. Based on the interpolation method, Lallemand & Luo [9] proposed an improved bounce-back scheme which has a higher order of accuracy as compared with the simple one and is suitable for the moving boundaries. Therefore, the non-slip conditions of the surface of moving sphere was treated by the improved bounce-back scheme in the present simulations. The momentum–exchange method [9] was used to compute the force and torque exerted on the sphere resulting from the motion of fluid. In addition, some fluid nodes may become solid nodes and some solid nodes may become fluid nodes due to the motion of sphere. To account for the effects of covered or uncovered fluid nodes, the method developed by Aidun et al. [10] was used here to compute the added force and torque exerted on the sphere. The motion of sphere is then determined by solving the Newton’s equations.

3. Problem

This work aims to shed light on the free motion and interaction of two unequal spheres under the action of gravity in a square tube. The schematic diagram of the problem is shown in Figure 1. The square tube with dimensions of \( L \times L \times H \) is filled with a fluid of density \( \rho \) and viscosity \( \nu \). Two spheres which have different densities (\( \rho_1 \) and \( \rho_2 \)) and diameters (\( d_1 \) and \( d_2 \)) are immersed in the fluid. Both spheres are assumed to be heavier than the fluid, i.e. \( \rho_1 > \rho \) and \( \rho_2 > \rho \). This means that the spheres will fall in the fluid once they are released from rest. Besides, this study considers the only case that both spheres are rising as a whole in the tube, suggesting that the conditions of \( \rho_1 < \rho_2 \) and \( d_1 > d_2 \) are held for all computations. Because a larger but heavier sphere will always leave a smaller but lighter sphere behind. The positions of the spheres are denoted as \( X \) (horizontal), \( Y \) (transversal) and \( Z \) (vertical). The subscripts 1 and 2 are used to represent the large and small spheres, respectively.

![Figure 1. Physical model and notations of the present problem.](image)
In the simulations the density and diameter of the large sphere are fixed. Therefore, the velocity scale of the present system is chosen as,

\[ U = \left( \frac{\rho_2}{\rho} - 1 \right) g d_1 \]  

(7)

Where \( g \) is the gravitational acceleration. The time scale is then defined by \( T = d_1/U \). The Reynolds number, denoted as \( Re = Ud_1/\nu \), is used to adjust the effect of fluid inertia in this work. Apart from \( Re \), another two dimensionless parameters are introduced to control the density and diameter ratios between the spheres, i.e. \( \lambda = \rho_2/\rho_1 \) and \( r = d_2/d_1 \).

In addition, a moving computational domain is employed to simulate an infinite tube. The top boundary is 18\( d_1 \) from the large sphere, whereas the bottom boundary is 12\( d_1 \) from it (i.e., the overall tube height is \( H = 30d_1 \)). The normal derivative of the velocity is zero at the top boundary, and the velocity at the bottom boundary is zero.

In the simulations, some parameters are fixed as follows: \( d_1 = 20, \rho_1 = 1.5, \rho = 1 \) and \( L = 5d_1 \). For all cases the large and small sphere are released from the initial positions of \((-d_1, 0, 12d_1)\) and \((d_1, 0, 12d_1)\), respectively. This indicates that initially the two spheres are symmetrical with respect to the tube axis in the center-line plane (i.e., \( y = 0 \)).

4. Results

The present three-dimensional computational code has been thoroughly validated in our previous work [7]. Therefore, this paper does not include the validation in order to save space. Figure 2 shows the time series of snapshots for the relative motion of the small sphere with respect to the large one for different density ratios at \( Re = 30 \) and \( r = 0.5 \). Note that the spheres are always settling in the center-line plane (i.e. \( y = 0 \)) where they are released from rest. As shown in Figure 2 (a, b), after the initial transients die down the spheres interact with each other exhibiting the DKT motion in a periodic manner when the density ratio is small, such \( \lambda = 1.56 \) and 1.6. This DKT motion is different from the usual ones in that the spheres never exchange their vertical positions. To provide insights into this issue, Figure 3 shows the instantaneous vorticity contours during one period for \( \lambda = 1.56 \), which correspond to Figure 2(a). The small sphere will be sucked into the wake of the large sphere once it moves to a position behind the large sphere [Figure 3(a)]. As a result, the small sphere approaches to the large sphere at an increasing speed because of reduced drag. The separation between the spheres is decreasing. This is known as “drafting”. After a while, the two spheres appear to contact with each other [Figure 3(b)]. This is the “kissing” process. In fact, this is not a real contact because there is a thin film between the spheres which generates a repulsive force (i.e., the lubrication force) to prevent the collision of the spheres. Then the small sphere begins to roll around the large sphere, as shown in Figure 3(c), which is referred to as the “tumbling”. After that the spheres are seen to separate [Figure 3(d)] and the cycle is repeated.

Figure 2. Relative motion of the small sphere with respect to the large one for different density ratios at \( Re= 30 \) (front view): (a) \( \lambda = 1.56 \), (b) \( \lambda = 1.6 \) and (c) \( \lambda = 1.7 \). Snapshots were taken every 1000 time steps. Note that the spheres are settling in the center-line plane (i.e., \( y = 0 \)) all the time. The arrows denote the orientations of the spheres at different times which are initially set to be zero (the same as below).
Figure 3. Instantaneous vorticity contours (front view) at different times during one period showing the periodic motion and interaction of the spheres: (a) drafting, (b) kissing, (c) tumbling and (d) separating. The parameters are chosen as $l = 1.56$, $r = 0.5$ and $Re = 30$.

In comparison with small values of $\lambda$ ($\lambda = 1.56$ or 1.6), a significant difference is seen for $\lambda = 1.7$, as shown in Figure 2(c). Instead of periodically oscillating, the small sphere is seen to remain steady after the initial transients die down. This gives rise to a stable staggered configuration of the spheres, which is similar to the observation made in two dimensions [6]. In addition, it is seen from Figure 2 that the small sphere rotates in counter clockwise direction whether it oscillates or not. In particular, the large sphere is seen to rotate in the same direction at a lower speed (not clear in the figure). This observation is similar to that in two dimensions [6].

Figure 4. Time history of the horizontal positions of both spheres for $\lambda = 1.6$ at $Re = 30$. Note that $X_1' = X_1/d_1$, $X_2' = X_2/d_1$ and $t' = t/T_0$ (the same as below).

Figure 5. Time history of the differences in the horizontal and vertical positions of the spheres for the same parameters as those in Figure 4. Note that $\Delta X' = X_2' - X_1'$ and $\Delta Z' = Z_2' - Z_1'$. 
Figure 4 shows the time history of the horizontal positions of the spheres for $\lambda = 1.6$ at $Re = 30$. The results are normalized in this manner: $X_1' = X_1/d_1$, $X_2' = X_2/d_1$ and $t' = t/T_0$. It is seen that the small sphere oscillates almost as strongly as the large sphere in the horizontal direction (see the amplitudes of both $X_1'$ and $X_2'$). Furthermore, Figure 4 indicates that the spheres oscillate 180 degree out of phase with each other because $X_1'$ reaches its maximum when $X_2'$ reaches its minimum and vice versa. To investigate this matter further, Figure 5 shows the time history of the differences in the horizontal and vertical positions of the spheres, i.e. $\Delta X' = X_2' - X_1'$ and $\Delta Z' = Z_2' - Z_1'$. It is seen that the amplitude of $\Delta Z'$ is almost twice that of $\Delta X'$, suggesting that the spheres oscillate much strongly in the vertical (gravity) direction. This is different from the observation made for the circular cylinders [6]. The primary reason for this difference is that the wake effect of a sphere is stronger than that of a cylinder at the same Reynolds number.

For large values of $r$ (e.g., $r = 0.75$ or 0.9), another stable staggered configuration of spheres is seen, as shown in Figure 6. In comparison with Figure 2(c), the small sphere moves to a position below the large sphere this time. Note that this configuration is only observed for $r \geq 0.75$. Furthermore, it is interesting to find that both spheres rotate clockwise though the speed of rotation is much bigger for the large sphere. This rotation is somewhat “abnormal” for the small sphere because it seems that the small sphere is rolling up when it falls in the tube.

The effects of the Reynolds number may be significant to the motion of the spheres. To check this some computations were performed at $Re = 15$. Figure 7 shows the relative motion of the spheres for $r= 0.5$ at different $\lambda$, which is similar to Figure 2. After the initial transients disappear the spheres may
undergo periodic motion or reach a steady state according to the value of $\lambda$. It is also seen that the spheres oscillate more strongly at high $Re$ (see Figure. 2) owing to the strong inertia of fluid. In particular, a significant difference is seen at $Re = 15$ when $\lambda$ is small, as illustrated in Figure. 7(a), which shows an inverse “tumbling” during the initial transients. This unusual phenomenon gives rise to the fact that the small sphere is locating on the left of the large sphere.

5. Conclusion
The three-dimensional lattice Boltzmann method was used to simulate the sedimentation of two unequal spheres in a square tube at small Reynolds numbers. The density and diameter ratios of the spheres were taken into account. It has been shown that the spheres may exhibit the repeated DKT motion when the density ratio is small. In particular, a stable staggered configuration is seen when the density ratio is large, for which the small sphere moves to a position above or below the large sphere at small or large diameter ratios. In addition, the spheres rotate in the same direction when this staggered configuration is formed. At low Reynolds numbers, the small sphere may undergo an inverse “tumbling” process when the density ratio is small. This phenomenon is unusual because it results in the fact that the spheres exchange their horizontal positions.

Acknowledgements
This work was supported by the National Natural Science Foundation of China (11632016 and 11972336).

References
[1] A. Fortes, D.D. Joseph, T.S. Lundgren, Nonlinear mechanics of fluidization of beds of spherical particles. J. Fluid Mech. 177 (1987) 467–483.
[2] J. Feng, H.H. Hu, D.D. Joseph, Direct simulation of initial value problems for the motion of solid bodies in a Newtonian fluid. Part 1. Sedimentation. J. Fluid Mech. 261 (1994) 95–134.
[3] W. Fornari, M. Ardekani, L. Brandt, Clustering and increased settling speed of oblate particles at finite Reynolds number. J. Fluid Mech. 848 (2017) 696–721.
[4] C. K. Aidun and E. J. Ding, 2003 Dynamics of particle sedimentation in a vertical channel: period-doubling bifurcation and chaotic state. Phys. Fluids. 15 (2003) 1612–1621.
[5] R. Verjus, S. Guillou, A. Ezersky, J.-R. Angilella, Chaotic sedimentation of particle pairs in a vertical channel at low Reynolds number: multiple states and routes to chaos. Phys. Fluids 28 (2016) 123303.
[6] D. M. Nie and J. Z. Lin, 2019 Discontinuity in the sedimentation system with two particles having different densities in a vertical channel. Phys. Rev. 99 (2019) 053112.
[7] D. M. Nie and J. Z. Lin, Simulation of sedimentation of two spheres with different densities in a square tube J. Fluid Mech. 896 (2020) A12.
[8] Y. H. Qian, Lattice BGK models for Navier–Stokes equation. Europhys. 17 (1992) 479–484.
[9] P. Lallem and L. S. Luo, Lattice Boltzmann method for moving boundaries. J. Comput. Phys. 184 (2003) 406–421.
[10] C.K. Aidun, Y. Lu, E. Ding, Direct analysis of particulate suspensions with inertia using the discrete Boltzmann equation. J. Fluid Mech. 373 (1998) 287–311.