NUMERICAL INVESTIGATION OF A CAPSULE-SHAPED PARTICLE SETTLING IN A VERTICAL CHANNEL

by

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Short paper
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The previously developed lattice Boltzmann – direct forcing/fictitious domain method is improved by introducing a multiple-relaxation-time model, and a detailed investigation of sedimentation of a capsule-shaped particle settling in a channel is carried out. The effects of blockage ratio on the sedimentation pattern at low Reynolds numbers are studied. It concludes that for a narrow channel, besides vertical and horizontal pattern, there exists another sedimentation pattern named inclined pattern. Through a large amount of simulations, two critical lines are obtained, which divide the three patterns based on the critical values of density ratio.

Key words: *capsule-shaped, lattice Boltzmann method, sedimentation, simulation*

Introduction

Solid particles immersed in a viscous fluid lead to a two-phase flow problem. It requires the development of coupled fluid-flow and particle-motion computational methods to study the dynamics of individual particles. The direct numerical simulation (DNS) is an excellent tool to investigate the motion of colloidal particles. So far the largest and maybe the most realistic suspension simulations have been performed with the lattice Boltzmann method (LBM) [1-5] that appears to be advocated as an effective computational tool for the simulations of particle suspensions. Recently, Nie *et al*. [6] proposed a single-relaxation-time (SRT) based on lattice Boltzmann direct forcing/fictitious domain (LB-DF/FD) method for the simulation of particle suspensions, which was derived from SRT-LBM coupled with DF/FD method. It has been shown that LB-DF/FD is capable of dealing with non-spherical particle's motion [7]. The study of the motion of non-spherical particles in a viscous fluid has a long history, for example, cylindrical particles [8-11] and elliptical particles [12-14]. Feng *et al*. [12] demonstrated that an ellipse which settles between parallel walls will translate to the center of the channel due to wall effects and orient itself so that its major axis is orthogonal to the direction of gravity for any initial configuration. They grouped the behavior of the ellipse into four different regimes based on the Reynolds number which is up to 345. Accordingly, Huang *et al*. [13] showed that an ellipse which settles in a Newtonian fluid will turn vertical when the Reynolds number is below a critical value. Recently, Xia *et al*. [14] studied the dynamics of a single elliptical particle settling in a long narrow channel using a multi-block lattice Boltzmann method.

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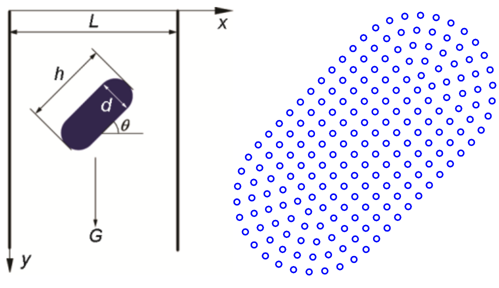
However, very few study focus on the capsule-shaped particles. In oral drug delivery system, sedimentation analysis provides a potentially powerful tool for the investigation of many phenomena relevant to pharmaceutical sciences. Furthermore, the dropping method for preparation of soft capsules has been known as one of the most popular methods to date. In this method, the sedimentation velocity of the soft capsule is important for the production. As a DNS work, it is hoped the present study will help understanding the dynamics of a capsule-shaped particle in the sedimentation. In previous study [15], we focus on the effects of the capsule-particle orientation and particle/fluid density ratio on the flow patterns during sedimentation. We also have conducted a detailed study on the effects of density ratio on the transition from vertical mode to horizontal mode [15]. In this study, we mainly focus on the effects of blockage ratio on the flow patterns at low Reynolds numbers. Furthermore, we also aim to improve the previous single-relaxation-time based LB-DF/FD method by introducing a multiple-relaxation-time (MRT) model.

The MRT model is the most general form derived from the linearized collision model within the theoretical framework of the LB equations and kinetic theory – it includes all possible degrees of freedom to optimize the LB equations, and it has been shown to be superior over the SRT model in terms of accuracy, stability, and computational efficiency [16].

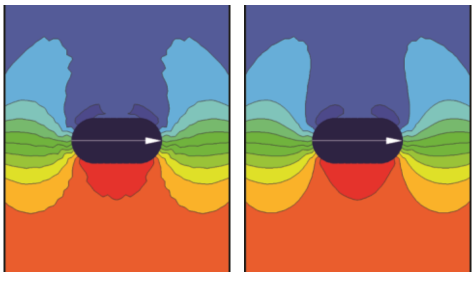
Numerical model

In this work we introduce a MRT model into the LB-DF/FD method. For D2Q9 lattice model used in this work, the MRT model includes nine non-negative relaxation rates, while the SRT model includes only one. For the sake of saving space, a detailed description of MRT model is not explained here, which can be found in [16]. The problem is described in fig. 1. The initial orientation θ_0 is kept $\pi/4$ unless otherwise specified. We introduce a fluid-particle density ratio $\gamma = (\rho_p - \rho_f)/\rho_f$ and a blockage ratio $\beta = L/h$. The arrangement of Lagrangian nodes inside the particle is shown in fig. 1(b).



(a) (b)

Figure 1. Problem description
(a) flow and particle, (b) arrangement of nodes



(a) (b)

Figure 2. Pressure distribution
(a) SRT, (b) MRT

Results and discussions

As shown in fig. 2, where the parameters are $\beta = 3$, $\gamma = 1.5\cdot10^{-3}$ and $\theta_0 = 0$, the general feature of pressure distribution of SRT model is similar to that of MRT model, while visible oscillation is observed in the SRT result which is hardly observed in the latter. For large blockage ratio such as $\beta = 5$, there exist two sedimentation patters: vertical pattern ($\theta = \pi/2$) and horizontal pattern ($\theta = 0$). However, if decreasing the blockage ratio β another sedimentation pattern named inclined pattern may take place. Figure 3 displays the inclined pattern. As shown in fig. 4 where β = 2.0, for γ_v = $3.9 \cdot 10^{-3}$ and γ_h = $8.1 \cdot 10^{-3}$ (subscript: *v*-vertical, *h*-horizontal), the particle sediments vertically and horizontally in the end. However, for $\gamma_v < \gamma < \gamma_h$, all results display inclined sedimentation pattern.

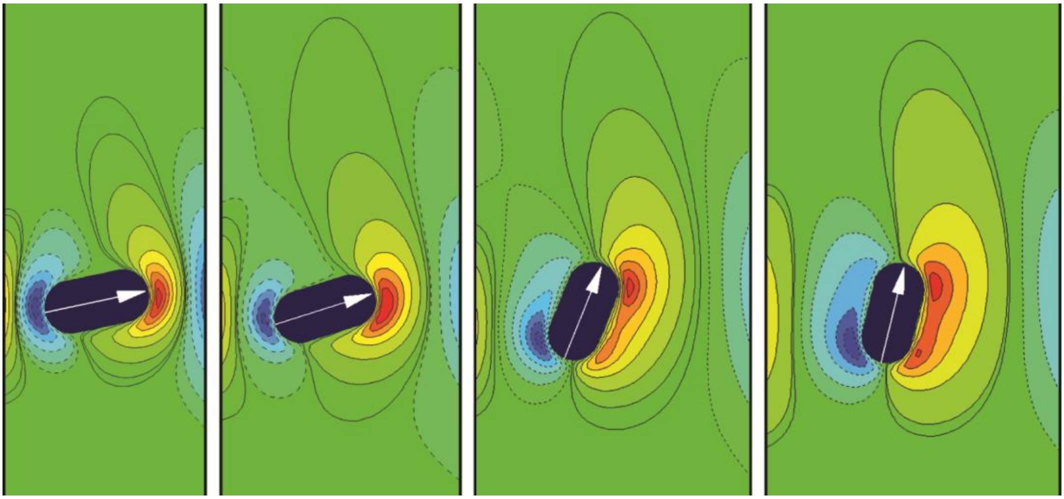


Figure 3. Inclined pattern for β = 2.0, 2.4, 2.8, and 3.0 (left to right)

Moreover, results also indicate that γ_v and γ_h are the critical values to divide the three patterns: $\gamma \leq \gamma_v$ (vertical), $\gamma_v < \gamma < \gamma_h$ (inclined) and $\gamma \geq \gamma_h$ (horizontal). For the vertical and horizontal pattern, as shown in fig. 5, corresponding to γ_v = $3.9 \cdot 10^{-3}$ and γ_h = $8.1 \cdot 10^{-3}$, the particle sediments along the channel centerline, while for the inclined pattern, the particle deviates from the centerline.

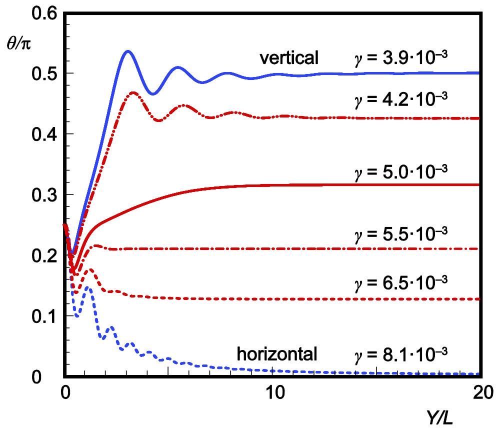


Figure 4. Evolution of particle orientation

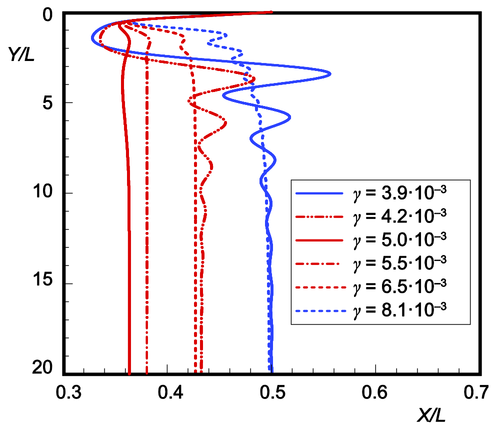


Figure 5. Evolution of particle trajectory

Furthermore, as density ratio increases the *X*-position of the particle decreases from 0.5 *L* firstly, and then increases to 0.5 *L*. More detail about the terminal states are shown in fig. 6, which further validates the above observations. The particle orientation always decreases as γ increases, while there exists a transition at about $\gamma = 5 \cdot 10^{-3}$ which obviously corresponds to the minimum value of the particle position.

Furthermore, there exist two linear dependence regions before and after the transition, as shown in fig. 6. Numerical results have shown that the critical values of γ_v and γ_h depend on the blockage ratio β. Through a large amount of simulations we conclude two critical lines which divide the three sedimentation patterns for different blockage ratio, as shown in fig. 7. Both of the values of γ_v and γ_h decrease with increasing β, leading to the smaller and smaller areas for the vertical pattern and inclined pattern. For the channel large enough such as $\beta = 4$ or 5, we can hardly find inclined pattern at all.

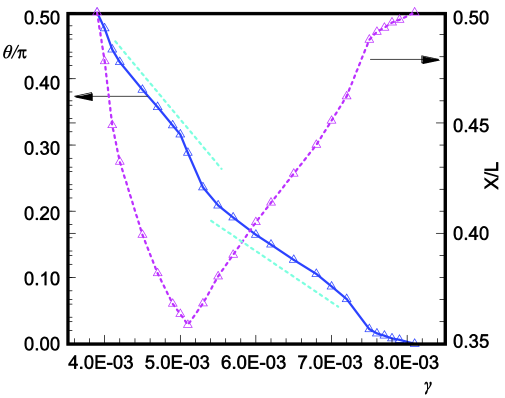


Figure 6. Terminal state of the particle

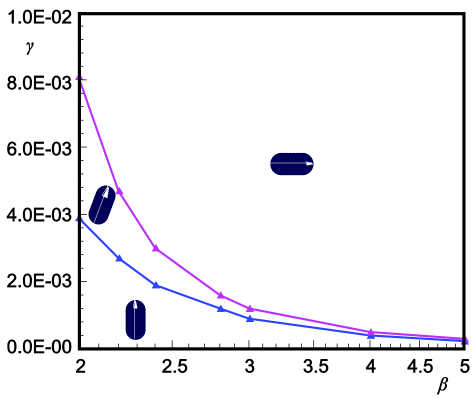


Figure 7. Critical lines dividing the patterns

Conclusions

We study the effects of blockage ratio on the capsule-shaped sedimentation patterns at low Reynolds numbers. Besides vertical and horizontal pattern, another sedimentation pattern, *i. e.* inclined pattern, is found when the blockage ratio is very low. We also obtain two critical lines which divide the three patterns based on critical values of density ratio.

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