Computers & Fluids 114 (2015) 110–120

Contents lists available at ScienceDirect

Computers & Fluids

journal homepage: www.elsevier.com/locate/compfluid

Numerical study on dynamic sorting of a compliant capsule with a thin shell

Huilin Ye, Haibo Huang *, Xi-yun Lu

Dept. of Modern Mechanics, Univ. of Sci. and Tech. of China, Hefei 230026, China

A R T I C L E   I N F O

Article history:
Received 4 December 2014
Received in revised form 10 February 2015
Accepted 28 February 2015
Available online 9 March 2015

Keywords:
LBM
LSM
Shear flow
Deformable particle
Narrow channel
Multi-particles

A B S T R A C T

Sorting compliant capsules is an interesting research topic. In this paper, a simple bifurcated micro-channel is used to sort the particles with different rigidities. The behavior of a compliant particle inside the channel is investigated numerically. The fluid flow and the particle's deformation are solved by Lattice Boltzmann Method (LBM) and Lattice Spring Model (LSM), respectively. The fluid and solid solvers are coupled through interpolated bounce-back scheme. Two benchmark problems are used to validate our method. One is the motion of a compliant capsule in a channel and the other is the deformation of a capsule inside a simple shear flow. The results are quantitatively consistent with those in literature. By taking advantage of the rotating of capsules in shear flow, a simple distinguished bifurcated micro-channel is proposed to sort capsules with different rigidities. In this micro-channel, the initial offset and shear stress induce the rotating and lateral migration of the capsule and flux ratio is determined by the outlet pressures. The competition between the effect of initial offset and flux ratio contributes to the sorting mechanism. Compared to other micro-channels with different geometrical models, present one is more convenient and may be more efficient to screen the microcapsule we want.

1. Introduction

In recent years, researchers are very interested in the deformation and motion behavior of a capsule enclosed with elastic membrane. A possible reason is that behavior of a capsule immersed in fluid is similar to that of a Red Blood Cell (RBC) suspended in plasma. As we know, the RBC plays important role in Oxygen transfer. The RBC is enclosed with lipid bilayer, which would protect the entity of the cell and afford the ability to deform. The RBC suspended in blood on one hand is driven to flow with the blood, on the other hand is deforming under the effect of the fluid enclosing it. Hence, understanding the motion and deformation behavior of the RBC is important. In blood diseases like cerebral malaria and sickle cell anemia, the rigidity of RBC would be affected much [1]. When the RBC goes through the constricted capillary tube, it may be unable to deform enough and in a certain condition, it may be destroyed by a little stimulant such as some impurity contained in blood. For the application of capsules, artificial capsules are often used in the pharmaceutical, cosmetics, and food industries. They could regulate the release of active substances and flavors. Because of the small size and fragility, measuring the mechanical properties of the membrane is very difficult.

Research in membrane hydrodynamics has achieved great success. It leads to numerous membrane constitutive laws. The simplest law is Hooke's law restricted to small deformations. Another is Mooney–Rivlin (MR) law which assumed the membrane is a very thin sheet [2]. In order to model the large deformations of RBC, Skalak et al. [3] proposed the Skalak (SK) Law. Some theoretical studies have been carried out. Barthes-Biesel [4] and Barthes-Biesel and Rallison [5] applied a regular perturbation to analyze cases where the deviation from spherical shape of the capsule is small or large. Barthes-Biesel et al. [6] also compared the effect of constitutive laws for two dimensional (2D) membranes. They found that after a continuous elongation, a capsule with a MR membrane bursts, while a capsule with a SK membrane would reach a steady state.

However, deformation of a RBC depends on not only the elastic of the membrane, but also the flow of fluid surrounding the RBC. The flows in complex geometry are difficult to be analyzed theoretically. To study the deformation, usually experimental and numerical methods are adopted. To investigate the deformation of a capsule in a simple shear flow, Chang and Olbricht [7] and Walter et al. [8] designed artificial capsules composed of different material. However, usually it is difficult to change the rigidity of the capsule in experiments. With the development of numerical methods and computers, more researchers carried out relevant numerical studies [9–17].

* Corresponding author.

http://dx.doi.org/10.1016/j.compfluid.2015.02.021
0045-7930/

Many numerical methods have been developed to solve both the deformation of the capsule and fluid flow. For example, Woolfenden and Blyth [18] used boundary element method to solve both the solid and fluid parts. Immersed-boundary method (IBM) is another simple but effective scheme to solve the flow problem. The IBM is introduced by Peskin [19], and developed by Feng et al. [20], which is usually used to simulate the moving boundary problem. In the scheme, the deformation of capsule and fluid flow are solved separately and the IBM is used to couple the solutions. For example, MacMeccan et al. [21] and Sui et al. [11] applied the finite element analysis (FEA) and Lattice Boltzmann Method (LBM) to solve the dynamics of the membrane and fluid flow, respectively. The IBM is adopted to couple the FEA and LBM. This method is able to simulate large numbers of capsules suspended in fluid efficiently [12]. Sui et al. [9,10] identified various types of motion for a capsule freely suspended in simple shear flow. For an initially spherical capsule, it would exhibit a steady "tank-treading" motion, wherein the capsule deforms into a stationary shape with a finite inclination with the flow direction and the membrane would rotate around the interior liquid. Keller and Skalak [22] analyzed the motion of a viscous ellipsoid and investigated the effect of viscosity ratio of the inner and outer fluids. They found the critical viscosity ratio for a capsule translating from tank-treading motion to tumbling motion. Abkarian et al. [23] and Skotheim and Secomb [24] found that lowering the shear rate of the external flow could trigger the transition from successive swinging mode to the pure tumbling mode. Kessler et al. [25] concluded a full phase diagram for varying shear rate and viscosity ratio.

For studies of capsules sorting, Alexeev et al. [26–28] came up with an idea about capsules that are driven by a shear flow going through compliant substrates or corrugated surfaces. The motion of capsules can be controlled through changing rigidity of the substrates or corrugated structure. Zhu et al. [29] designed a constricted pillar geometrical model to regulate the motion of capsule because the velocity of the capsule depends on the rigidity of the capsule. However, the above sorting methods are not easily and efficiently applied in engineering. Now, more and more researchers try to design different mechanism to sort capsules with different rigidity.

Here, taking advantage of "tank treading motion", we designed a simple bifurcated micro-channel to sort capsules with different rigidities. Through setting different pressures on the outlet boundaries of the device, we can control which sub-channel the capsules will enter into. In the literature, there are some studies on capsules' behavior near the bifurcation. Woolfenden and Blyth [18] conducted a two-dimensional elastic fluid-filled capsule through a channel with a side branch. The deformation experienced by the capsule near the junction of main channel and side branch is found to depend strongly on the branch angle, and the path selection of a cell at a branch junction can depend crucially on the capsule deformability [18]. Hyakutake et al. [30] and Barber et al. [31] used 2D bifurcation flow to investigate the blood cell behavior at microvascular bifurcations. They found the fractional particle flux to a daughter branch is almost similar to the fractional bulk flow to the same branch in high hematocrit. However, in low hematocrit, the fractional particle flux against the fractional bulk flow increases. Hence, in previous relevant studies, no one focused on sorting capsules using simple bifurcated micro-channel.

To evaluate the performance of the device we designed, we take a numerical study on the sorting mechanism. Our numerical method is based on that of Alexeev et al. [26]. Capsule is modeled as a fluid-filled elastic shell. The Lattice Spring Model (LSM) is used to solve the deformation of the shell [32–35]. This model is able to simulate the solid material constructed by isotropic homogeneous elastic medium [32]. In the model, discrete solid nodes are connected with linear springs. For the fluid flow, the LBM is used, which is an efficient solver for Navier–Stokes equations [36–38]. The interpolated bounce-back scheme is used to couple the fluid flow and deformation of the capsules. However, Omori et al. [14] has used the numerical test of tension-strain relations and the isotropic tension-area dilation relations for large deformation to demonstrate that the cross mesh type we used in our paper exhibits a strain-hardening behavior and strain-softening behavior,respectively. So we set the capsule's deformation relatively low ($Ca < 0.2$) in order to model the biological cell membranes which is local area incompressibility more closely.

In this paper, first the numerical methods about LBM and LSM are introduced briefly. Then the numerical method is validated by two benchmark problems. One is the motion of a compliant capsule in a channel and the other is the deformation of a capsule inside a simple shear flow. Finally, sorting mechanism of capsules with different rigidity through the bifurcated channel is explored.

2. Method

2.1. Lattice Boltzmann method

In our study, the fluid flow is solved using LBM. In the LBM, the Bhatnagar–Gross–Krook (BGK) approximation for the collision term is adopted [36]. In the lattice BGK method, a distribution function $f_i(\mathbf{x}, t)$ is introduced to implicitly represent all relevant properties of the fluid. This distribution function satisfies the following lattice Boltzmann equation [36]:

$$f_i(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)), \tag{1}$$

where $f_i(\mathbf{x}, t)$ is the density distribution function in the discrete velocity $\mathbf{e}_i$ direction. $f_i(\mathbf{x}, t)$ is functions of position $\mathbf{x}$ and time t. τ is a non-dimensional relaxation time which is related to the kinematic viscosity by $\nu = c_s^2(\tau - 0.5)\Delta t$. Usually in the LBM code, Eq. (1) is decomposed into two steps. One is the streaming step:

$$f_i(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) = f_i^+(\mathbf{x}, t), \tag{2}$$

the other is the collision step:

$$f_i^+(\mathbf{x}, t) = f_i(\mathbf{x}, t) - \frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)). \tag{3}$$

The equilibrium distribution function $f_i^{eq}(\mathbf{x}, t)$ can be calculated as [36]

$$f_i^{eq}(\mathbf{x}, t) = w_i\rho\left[1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{(\mathbf{u})^2}{2c_s^2}\right]. \tag{4}$$

In Eqs. (1) and (4), for the two-dimensional nine-velocity (D2Q9) model, $\mathbf{e}_i$s are given by [36]

$$[\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4, \mathbf{e}_5, \mathbf{e}_6, \mathbf{e}_7, \mathbf{e}_8] = c \cdot \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}.$$

In Eq. (4) the weighting coefficients $w_i = 4/9$, ($i = 0$), $w_i = 1/9$, ($i = 1, 2, 3, 4$), $w_i = 1/36$, ($i = 5, 6, 7, 8$). The lattice sound speed in the LBM [36] is $c_s = \frac{c}{\sqrt{3}}$ for the D2Q9 model, where $c = \frac{\Delta x}{\Delta t}$ is the ratio of lattice spacing Δx and time step Δt. Here, we define 1 lattice unit (Δx) as 1 *lu*, 1 time step (Δt) as 1 *ts*, and 1 mass unit as 1 *mu*.

In Eq. (4), ρ is the density of the fluid, which can be obtained from the zeroth order moment of f_i [36],

$$\rho = \sum_i f_i, \tag{5}$$

and ρ_0 is used to denote the average density of the fluid. The fluid velocity can be calculated through the first order moment of f_i [36],