Numerical Simulation of the Motion of Inextensible Capsules in Shear Flow Under the Effect of the Natural State

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Abstract. In this paper, a computational model for the natural state of an inextensible capsule has been successfully combined with a spring model of the capsule membrane to simulate the motion of the capsule in two-dimensional shear flow. Besides the viscosity ratio of the internal fluid and external fluid of the capsule, the natural state also plays a role for having the transition between two well known motions, tumbling and tank-treading (TT) with the long axis oscillates about a fixed inclination angle (a swinging mode), when varying the shear rate. Between tumbling and tank-treading, the intermittent behavior has been obtained for the capsule with a biconcave rest shape. The estimated critical value of the swelling ratio for having the intermittent transition behavior is less than 0.7, i.e., the capsules with rest shape closer to a full disk do not have the intermittent behavior in shear flow. The intermittent dynamics of the capsule in the transition region is a mixture of tumbling and TT with a swinging mode. Just like the motion of TT with a swing mode, which can be viewed as a tank-treading with an incomplete tumbling, the membrane tank-treads backward and forward within a small range during the tumbling motion.

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Key words: Natural state, tumbling, tank-treading with a swinging mode, intermittent region, capsule, shear flow.

1 Introduction

The dynamical behavior of deformable entities such as lipid vesicles, capsules, and red blood cells (RBCs) in flows has received increasing attention experimentally, theoretically, and numerically in recent years. Lipid vesicles [1–10], non-spherical capsules [11–15],...
and red blood cells [16–24] show phenomenologically similar behavior in shear flows, which are (i) an unsteady tumbling motion, (ii) a tank-treading rotation with a stationary shape and a fixed inclination angle with respect to the flow direction, and (iii) while tank-treading (TT), the long axis oscillates about a fixed inclination angle which is called swinging mode in [9] (but it is still called the tank-treading in [12]). The aforementioned motions depend on the shear rate, viscosity ratio between internal fluid and external fluid, membrane viscosity and other parameters. Noguchi and Gompper [7–9] have studied the dynamics of vesicles in simple shear flow using mesoscale simulations of dynamically triangulated surfaces. Vesicles are found to have a vacillating breathing mode when transiting from steady tank-treading to unsteady tumbling with increasing membrane viscosity or the shear rate. At the vacillating breathing mode, the main axis makes oscillation around the flow direction (around zero degree angle, but with large amplitude). In [9], they have developed a model based on the classical model of Keller and Skalak [11] (KS model) for the membrane to theoretically explain the vesicle motion. Using such model, they obtained the swinging mode and studied the dependency of transition between tumbling and TT with a swinging mode on the shear rate, the viscosity ratio of the membrane and the internal fluid, and the reduced volume [9]. Abkarian et al. [19] observed the intermediate motions at the transition from swinging to tumbling (resp., tumbling to swinging) by reducing (resp., increasing) the flow shear rate. A simplified model with a fixed elliptical shape for cell membrane has been studied to support their observations. In [12], Skotheim and Secomb introduced an elastic energy term based on the phase angle of the tank-treading rotation to the KS model. They observed tumbling, tank-treading (with a swinging mode), and the intermittent behavior at the transition between tumbling and tank-treading and analyzed the influence of the viscosity ratio, membrane elasticity, shape, and the shear rate on the motion of a capsule of either prolate or oblate shape. The both models considered in [12, 19] take into account the membrane elastic energy. Tsubota et al. [22] used a spring model fully coupled with fluid flow to study cell motion dependency on the natural state of membrane through the bending energy term in two-dimensional shear flow. When being at uniform natural state (i.e., all reference angles as defined in Section 2.1 are set to be the same), the cell appears to tank-tread with an inclination angle unchanged and independent of the preset value of reference angles. But when a biconcave resting shape is assumed as the natural state (called non-uniform state), the cell is observed to perform tumbling and tank-treading with a swinging mode. Tsubota et al. [22] believed that the intermittency between tumbling and TT with a swinging mode would occur in very narrow range of parameter space; but they did not obtain such intermittent region because, as discussed later in this paper, the swelling ratios of their cells are not small enough. The elastic energy term introduced by Skotheim and Secomb in [12] has a similar characteristics like the bending energy defined with a non-uniform state used by Tsubota et al. in [22] since both have their preferred rest states, which are preferred phase angles at zero and 180 degrees and a biconcave resting shape for Skotheim and Secomb’s model and Tsubota et al.’s model, respectively. In [14], Vlahovska et al. used perturbation approach to study the
motion of an almost spherical capsule in shear flow at the Stokes regime. Their reduced models are more general and have no restriction of the fixed shape on the capsule when comparing with the one used in [12]. Without the elastic energy introduced by Skotheim and Secomb in [12], Vlahovska et al. obtained the intermittent behavior when having deformation only in the shear plane and that the intermittent behavior disappears in Stokes flow for an almost spherical capsule which can deform in the vorticity direction. They concluded that the intermittency is an artifact of the shape preservation. But they did not analyzed the cases of capsules of more interesting shapes such as a biconcave shape.

In [10], Zhao and Shaqfeh have performed direct numerical simulation of a lipid vesicle under Stokes flow conditions in simple shear flow. The lipid membrane is modeled as a two-dimensional incompressible fluid with Helfrich surface energy in response to bending deformation. The critical viscosity ratios for the transition from tank-treading to vacillating breathing, and eventually tumbling motions have been studied. In [21], Fedosov et al. used a two-dimensional spring network with the natural state in their bending energy term to model red blood cell membrane. They obtained the intermittent region of mixed dynamics in shear flow for the cases of the viscosity ratio $\lambda$ greater than or equal to 1.

In this paper, a computational model for the natural state of an inextensible capsule has been successfully combined with a spring model of the capsule membrane, an immersed boundary method, operator splitting and finite element methods to simulate the motion of the capsule in two-dimensional shear flow. The capsule motion in simple shear flow has been analyzed via direct numerical simulations under the effect of the natural state. With the results of the go-and-stop test on the proposed models, the membrane point at the rim goes back to the rim and the membrane point from dimple goes back to the dimple. The restriction of the non-deformability (i.e., the fixed shape considered in [12]) has also been relaxed and a fully interaction of the fluid and capsule in two dimensional shear flow has been considered in this article. Furthermore, we have studied the dependency of the capsule motion on the capillary number $C_a = \mu \gamma R_0^3 / B$, where $\mu$, $\gamma$, $R_0$, and $B$ stand for the fluid viscosity, the shear rate of fluid flow based on the gradient of the velocity at the wall, the effective radius of the capsule and the bending modulus, respectively. We have obtained that the swelling ratio of the capsule does have its effect on the intermittent region. The intermittent behavior of mixed dynamics between tumbling and TT with a swinging mode of the capsule with a biconcave rest shape has been obtained in a narrow range of the capillary number. For the capsule of swelling ratio greater than 0.6, it is almost impossible to capture the intermittent region computationally since the size of the capillary number range for such region is about zero if it exists. Our results are consistent with the results obtained by Tsubota et al. in [22] since the cells used in their simulations have the swelling ratio of 0.7. In [12], Skotheim and Secomb’s membrane elastic energy term, based on the phase angle, has preferred phase angles at zero and 180 degrees; i.e., the point at the rim likes to go back to the rim. Our elastic energy term based on the non-uniform natural state also has such preference. Through the preferred phase angle (please also see Fig. 4), we link our cases of one dimensional
(1D) membrane in two-dimensional (2D) flow with the 2D membrane discussed in [12] by Skotheim and Secomb.

The contents of this article are as follows: We discuss the models and numerical methods in Section 2. In Section 3, we first show validations and also carry out the go-and-stop experiments on the model to illustrate the effect the natural state on the preferred rest shape. Then the dynamics of an inextensible capsule under the effect of the natural state in shear flow are studied at different values of the capillary number. The conclusions are summarized in Section 4.

2 Models and numerical methods

A capsule with non-spherical rest shape is suspended in a domain $\Omega$ filled with a fluid, as in Fig. 1, which is incompressible and Newtonian. The inclination angle $\theta$ and phase angle $\phi$ are defined as in Figs. 1(b) and 1(c), respectively (see Remark 3.1 for more detail). For some $T > 0$, the governing equations for the fluid-capsule system are the Navier-Stokes equations

$$
\rho_f \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f}_B \quad \text{in} \quad \Omega \times (0, T),
$$

$$
\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega \times (0, T),
$$

with the following boundary and initial conditions:

$$
\mathbf{u} = \mathbf{g} \quad \text{on} \quad \Gamma \quad \text{and is periodic in the } x_1\text{-direction},
$$

$$
\mathbf{u}(x, 0) = \mathbf{u}_0(x) \quad \text{in} \quad \Omega.
$$

Figure 1: (Color online) Schematic diagram of (a) an inextensible biconcave capsule in shear flow with the computational domain $\Omega$, (b) the inclination angle $\theta$, and (c) the phase angle $\phi$. 
where \( u \) and \( p \) are the fluid velocity and pressure, respectively, \( \rho_f \) is the fluid density, and \( \mu \) is the fluid viscosity, which is assumed to be constant for the entire fluid. In (2.1), \( f_B \) accounts for the force acting on the fluid/capsule interface, and \( \Gamma \) is the top and bottom walls of \( \Omega \). The boundary condition on \( \Gamma \) in (2.3) is \( g = (U,0)^t \) on the top wall of \( \Omega \) and \( g = (-U,0)^t \) on the bottom wall of \( \Omega \) for simple shear flow. In (2.4), \( u_0(x) \) is the initial fluid velocity.

2.1 Elastic spring models

An elastic spring model similar to the one used in [22] is considered in this paper to describe the deformable behavior and elasticity of capsules. Based on this model, the capsule membrane can be viewed as membrane particles connecting with the neighboring membrane particles by springs, as shown in Fig. 2. Energy stores in the spring due to the change of the length \( l \) of the spring with respect to its reference length \( l_0 \) and the change in angle \( \theta \) between two neighboring springs. The total energy per unit thickness of the capsule membrane, \( E = E_l + E_b \), is the sum of the one for stretch and compression and the one for the bending which, in particular, are

\[
E_l = \frac{k_l}{2} \sum_{i=1}^{N} \left( \frac{l_i - l_0}{l_0} \right)^2, \quad E_b = \frac{k_b}{2} \sum_{i=1}^{N} \tan^2 \left( \frac{\theta_i - \theta_0^i}{2} \right).
\]  

In Eq. (2.5), \( N \) is the total number of the spring elements, and \( k_l \) and \( k_b \) are spring constants for changes in length and bending angle, respectively. The set of reference angles \( \{\theta_0^i\}_{i=1}^{N} \) corresponds to a preset natural state, where \( \theta_0^i = \text{constant} \) for all \( i \) corresponds to a uniform natural state, and otherwise a nonuniform natural state.

To obtain a specified initial shape, which also serve as the reference shape at rest for the natural state, we have used the \( E_l \) and \( E_b \) given in Eq. (2.5) with \( \theta_0^i = 0 \) for \( i = 1, \cdots, N \). The capsule is assumed to be a circle of radius \( R_0 = 2.8 \mu m \) initially and then it is discretized into \( N = 76 \) membrane particles so that 76 springs of the same length are formed by connecting the neighboring particles. The shape change is stimulated by
Reducing the total area of the circle through a penalty function

$$\Gamma_s = \frac{k_s}{2} \left( \frac{s - s_e}{s_e} \right)^2,$$

(2.6)

where $s$ and $s_e$ are the time dependent area of the capsule and the targeted area of the capsule, respectively, and the total energy per unit thickness is modified as $E + \Gamma_s$. Based on the principle of virtual work the force per unit thickness acting on the $i$th membrane particle now is

$$F_i = -\frac{\partial (E + \Gamma_s)}{\partial r_i},$$

(2.7)

where $r_i$ is the position of the $i$th membrane particle. When the area is reduced, each membrane particle moves on the basis of the following equation of motion:

$$m \frac{d^2 r_i}{dt^2} + \gamma \frac{dr_i}{dt} = F_i.$$

(2.8)

Here $m$ and $\gamma$ represent the membrane particle mass and the membrane viscosity of the capsule. The position $r_i$ of the $i$th membrane particle is solved by discretizing Eq. (2.8) via a second order finite difference method. The total energy stored in the membrane decreases as the time elapses. The final shape of the capsule is obtained as the total energy is minimized and such shape is at a stress-free state. Fig. 3 presents final resting shapes for different values of the swelling ratio $s^* = s_e / (\pi R_0^2)$, which are about the same as those obtained by Kaoui et al. [33]. Based on the final shape, which is also the shape of natural state and the initial shape for fluid-capsule interaction, the reference angle between two neighboring springs at the $i$th node is $\theta_0^i$ for $i = 1, \cdots, N$. Our bending term in Eq. (2.5) is similar to the bending energy used by Fedosov et al. (e.g., see [21]) which is based on a two-dimensional spring network with the natural state as follows

$$V_{\text{bending}} = k_b \sum_{i=1}^{N_s} [1 - \cos(\theta_i - \theta_0^i)] = k_b \sum_{i=1}^{N_s} 2 \sin^2 \left( \frac{\theta_i - \theta_0^i}{2} \right),$$

where $N_s$ is the total number of the springs, $\theta_i$ is the angle between two triangles sharing the $i$th spring as their edges and $\theta_0^i$ is the angle of uniform natural state. The term $E_b$ defined in Eq. (2.5) is a discrete analogue of the elastic energy introduced by Skotheim and Secomb in [12]. The pictures of the normalized $E_b$ and the normalized elastic energy $\sin^2 \phi = 0.5 - 0.5 \cos 2\phi$ used in [12] versus the phase angle $\phi$ are shown in Fig. 4, in which the graph of the normalized term $E_b$ is obtained by rotating the mass nodes on the membrane of a given fixed shape in a clockwise manner. Both of them have preferred phase angles at zero and 180 degrees. We also modify the bending energy per unit thickness to a weighted sum of both uniform and nonuniform natural states to have a weaker effect of the nonuniform natural state:

$$E_b = \frac{k_b}{2} \left( (1 - \alpha) \sum_{i=1}^{N} \tan^2 \left( \frac{\theta_i}{2} \right) + \alpha \sum_{i=1}^{N} \tan^2 \left( \frac{\theta_i - \theta_0^i}{2} \right) \right).$$

(2.9)
Figure 3: The final resting shape for different swelling ratios \( s^* = 0.481, 0.6, 0.7, 0.8, 0.9, 0.95, 1.0 \) (from left to right).

Figure 4: The comparison of the normalized elastic energy term used in ref. [11] (solid line) and the discrete energy in (2.5) versus the phase angle \( \phi \) for two different initial shapes at rest: swelling ratio \( s^* = 0.481 \) (left) and 0.9 (right). The elastic spring model of the capsule membrane.

Here, \( \alpha \) indicates the weight of the nonuniform natural state.

In Eqs. (2.5), (2.6) and (2.9), \( E_l, E_b, \) and \( \Gamma_s \) represent energies [N m] per unit thickness of 1 m, and thus the units of \( k_l, k_b, \) and \( k_s \) are Newton [N]. In this paper, we only consider the capillary number instead of shear rate, because it is the key number to determine the behavior of capsules in two-dimensional flow. The values of parameters for modeling capsules are as follows: The spring constant is \( k_l = 5 \times 10^{-8} \) N, the penalty coefficient is \( k_s = 10^{-5} \) N, and the bending constant is \( k_b = 5 \times 10^{-10} \) N. Using the above chosen parameter values, the area of the initial shape of the capsule has less than 0.001% difference from the given equilibrium area \( s_e \), and the length of the capsule perimeter of the initial shape has less than 0.005% difference from the circumference of the initial circle.

2.2 Immersed boundary method

The immersed boundary method developed by Peskin, e.g., [25–27], is employed in this study because of its distinguished features in dealing with the problem of fluid flow interacting with a flexible fluid/structure interface. Over the years, it has demonstrated its CFD capability including blood flow simulations. Based on the method, the boundary of the deformable structure is discretized spatially into a set of boundary nodes. The force located at the immersed boundary node \( r_i = (r_{i,1}, r_{i,2}) \) affects the nearby fluid mesh.
The velocity of the immersed boundary node $r_i$ is also affected by the surrounding fluid and therefore is enforced by summing the velocities at the nearby fluid mesh nodes $x$ weighted by the same discrete $\delta$-function:

$$U(r_i) = \sum h^2 u(x) D_h(x - r_i) \quad \text{for } |x - r_i| \leq 2h.$$  \hfill (2.13)

After each time step, the position of the immersed boundary node is updated by advection through a locally interpolated fluid velocity

$$r_i^{n+1} = r_i^n + \Delta t U(r_i^n).$$  \hfill (2.14)

2.3 Computational methods

The weak formulation for the capsule-flow problem (2.1)-(2.4) in a channel reads as follow:

For a.e. $t > 0$, find $u(t) \in (H^1(\Omega))^2$, $p(t) \in L^2_0$, such that

$$\begin{cases}
\rho \int \Omega \left[ \frac{\partial u}{\partial t} + (u \cdot \nabla) u \right] \cdot v \, dx + \mu \int \Omega \nabla u : \nabla v \, dx - \int \Omega p \nabla \cdot v \, dx \\
= \int \Omega f_B \cdot v \, dx, \forall v \in W_{0,p},
\end{cases}$$  \hfill (2.15)

$$\int \Omega q \nabla \cdot u \, dx = 0, \forall q \in L^2(\Omega),$$  \hfill (2.16)

$$u(x,0) = u_0(x) \text{ in } \Omega,$$  \hfill (2.17)

$$u = g \text{ on } \Gamma,$$  \hfill (2.18)

with

$$W_{0,p} = \{ v | v \in (H^1(\Omega))^2, v = 0 \text{ on } \Gamma \text{ and is periodic in the } x_1 \text{ direction} \},$$

$$L^2_0 = \{ q | q \in L^2(\Omega), \int \Omega q \, dx = 0 \}.$$
Concerning the finite element based space approximation of \( \{u, p\} \) in problem (2.15)-(2.18), we use the \( P_1 \)-iso-\( P_2 \) and \( P_1 \) finite element approximation (e.g., see [28, Chapter 5]). Suppose that a rectangular computational domain \( \Omega \subset \mathbb{R}^2 \) is chosen with length \( L \), \( h \) is a space mesh size, \( \mathcal{T}_h \) is a uniform finite element triangulation of \( \Omega \) for velocity, and \( \mathcal{T}_{2h} \) is a twice coarser uniform triangulation for pressure. Let \( P_1 \) be the space of polynomials in two variables of degree \( \leq 1 \), we introduce the finite dimensional spaces:

\[
W_{h, g} = \{v_h | v_h \in C^0(\overline{\Omega}), v_h|_T \in P_1 \times P_1, \forall T \in \mathcal{T}_h, v_h = g \text{ on } \Gamma \text{ and is periodic in the } x_1 \text{ direction with period } L \},
\]

\[
W_{h, 0} = \{v_h | v_h \in C^0(\overline{\Omega}), v_h|_T \in P_1 \times P_1, \forall T \in \mathcal{T}_h, v_h = 0 \text{ on } \Gamma \text{ and is periodic in the } x_1 \text{ direction with period } L \},
\]

\[
L^2_h = \{q_h | q_h \in C^0(\overline{\Omega}), q_h|_T \in P_1, \forall T \in \mathcal{T}_{2h}, q_h \text{ is periodic in the } x_1 \text{ direction with period } L \},
\]

\[
L^2_{h, 0} = \{q_h | q_h \in L^2_h, \int_{\Omega} q_h dx = 0 \}.
\]

Then we apply the Lie's scheme [28, 29], which is first-order accurate, to Eqs. (2.15)-(2.18) with the backward Euler method in time for some subproblems and obtain the following fractional step subproblems (some of the subscripts \( h \) have been dropped):

\( u^0 = u_0 \) is given; for \( n \geq 0 \), \( u^n \) being known, we compute the approximate solution via the following fractional steps:

1. Solve

\[
\begin{align*}
\rho \int_{\Omega} \frac{u^{n+1/3} - u^n}{\Delta t} \cdot v dx - \int_{\Omega} p^{n+1/3}(\nabla \cdot v) dx &= 0, \quad \forall v \in W_{h, 0}, \\
\int_{\Omega} q \nabla \cdot u^{n+1/3} dx &= 0, \quad \forall q \in L^2_h, \\
u^{n+1/3} &\in W_{h, g}, \quad p^{n+1/3} \in L^2_{h, 0}.
\end{align*}
\]

(2.19)

2. Update the position of the membrane by (2.13) and (2.14) and then compute the force \( f_B \) on the fluid/capsule interface by (2.7) and (2.10).

3. Solve

\[
\begin{align*}
\int_{\Omega} \frac{\partial u(t)}{\partial t} \cdot v dx + \int_{\Omega} (u^{n+1/3} \cdot \nabla) u(t) \cdot v dx &= 0 \text{ on } (t^n, t^{n+1}), \quad \forall v \in W_{h, 0}, \\
u(t^n) &= u^{n+1/3}, \\
u(t) &\in W_{h, g} \text{ on } (t^n, t^{n+1}),
\end{align*}
\]

(2.20)

and set \( u^{n+2/3} = u(t^{n+1}) \).

4. Finally solve

\[
\begin{align*}
\rho \int_{\Omega} \frac{u^{n+1} - u^{n+2/3}}{\Delta t} \cdot v dx + \mu \int_{\Omega} \nabla u^{n+1} : \nabla v dx &= \int_{\Omega} f_B \cdot v dx, \quad \forall v \in W_{h, 0}, \\
u^{n+1} &\in W_{h, g}.
\end{align*}
\]

(2.21)
Remark 2.1. In simulations, the capsule with the initial rest shape obtained in Section 2.1 is suspended in a fluid which has a density $\rho = 1.00 \text{ g/cm}^3$ and a dynamical viscosity $\mu = 0.012 \text{ g/(cm s)}$. The viscosity ratio of the inner and outer fluid of the capsule membrane is fixed at 1.0. The degenerated quasi-Stokes problem (2.19) is solved by a conjugate gradient method (see, e.g., [28]). System (2.20) is an advection type subproblem and is solved by a wave-like equation method, which is described in detail in [28, 30]. Problem (2.21) is a classical discrete elliptic system. The subproblems (2.19) and (2.21) have been solved on a uniform and structured triangular mesh so that the specialized fast solver, such as FISHPAK by Adams et al. [31], can be used. For simulating the interaction of multiple capsules in fluid flow, we may need to apply a Morse type potential function (e.g., see [32]) to prevent the overlapping of capsules.

3 Numerical results and discussion

3.1 Validation

3.1.1 An inextensible capsule tank-treading in the shear flow

First, we present the simulating results of an inextensible capsule with uniform natural state (i.e., $a = 0$ in Eq. (2.9) and $\theta_i^0 = 0$, for $i = 1, \cdots, N$) suspended in a linear shear flow with shear rate $\gamma = 500/\text{s}$. The dimensions of the computational domain are $100\mu\text{m} \times 7\mu\text{m}$ and $100\mu\text{m} \times 14\mu\text{m}$. The two degrees of confinement are $R_0/w = 0.8$ for the narrower domain and 0.4 for the wider domain, respectively, where $w$ is the height of the channel. The grid resolution for the computational domain is 80 grid points per $10 \mu\text{m}$. The time step $\Delta t$ is $1 \times 10^{-4}\text{ms}$. The initial velocity of the fluid flow is zero everywhere and the initial positions of the mass center of the capsule are the center of both domains. In both wider and narrower domains, the capsule performs a steady tank-treading motion with a fixed inclination angle which depends on the swelling ratio $s^*$ and degree of confinement. The steady inclination angles and the membrane tank-treading velocities of two different degrees of confinement for four values of the swelling ratio $s^* = 0.6, 0.7, 0.8$ and 0.9 are presented in Fig. 5, which show good agreement with the results by Kaoui et al. [33]. The inclination angle increases monotonically for both two degrees of confinement with increasing the value of the swelling ratio $s^*$. For the same swelling ratio, the bigger is the degree of confinement, the smaller is the steady inclination angle. On the other side, the tank-treading velocity (scaled by $\gamma R_0/2$ as in [33]) has the increases almost linearly with respect to increasing of swelling ratio in the narrower channel, while in the wider domain the increasing of tank-treading velocity has slowed down until it arrives almost maximum around $s^* \sim 0.9$. The same qualitative tendency is given in [6,11,16,33,35]. Here the tank-treading velocity is obtained by $2\pi R_0/T$ where $T$ is the time for a membrane particle to go through entire circumference of the capsule.

We also keep track of the area and the perimeter of the capsule during the simulations. The variation is less than 0.1% in the area and 0.5% in the perimeter. Our model does keep capsules as an inextensible one in simulations.
3.1.2 A go-and-stop experiment for the shape recovery

A capsule or cell is said to have the shape memory if after stopping the flow, the deformed one will go back to its initial shape with any part of the membrane regaining its original position, i.e., the rim always returns to the rim and the dimple is always back to the dimple. To show that the capsule with a nonuniform natural state modeled by (2.5)-(2.7) and (2.9) does have the shape memory property, we have simulated several cases of the go-and-stop.

Fig. 6 shows a capsule with $\alpha = 1$ (fully non-uniform) of the swelling ratio $s^* = 0.481$ suspended in a simple shear flow at the capillary number $Ca = 6.365$ in a channel of the length $80\mu m$ and width $20\mu m$. The top and bottom walls of the channel are driven at the same speed in opposite directions as shown in Fig. 1(a). The capsule is at its reference shape at time $t = 0$ s, with a membrane particle at the dimple marked by a small “o”. At the beginning, the capsule performs a tank-treading motion with a swinging mode and the marked position tank-treads along the membrane as in Fig. 6 (top). We then suddenly stop the motion of two walls by setting the boundary conditions on them equal to zero, and observe (in Fig. 6 (middle)) that the capsule first returns to the biconcave shape very quickly and then the marked position tank-treads back to its initial location on the membrane, this behavior is first observed in experiments by T. M. Fischer in [24]. The capsule energy, plotted in Fig. 6 (bottom), is minimized when the capsule is at its natural state. During TT with a swinging mode, the capsule energy changes periodically with the period equal to the half of the period of oscillation due to the symmetry of the capsule natural state. After stopping the motion of two walls, the capsule energy returns to the one at its natural state. At lower $\alpha$ values, we get the same behavior of the rim back to the rim and the dimple back to the dimple after the walls stopped moving, as shown in Fig. 7 for $\alpha = 0.05$. For $\alpha = 0$ (see Fig. 8), the tank-treading motion stops right after the wall motion stops; but the membrane particle from dimple does not go back to the dimple.
We have also considered the cases with $\alpha = 1$, 0.05 and 0 at the same capillary number $C_a = 4.5467$ to compare the recovery of the biconcave shape. Fig. 9 presents the snapshots of the shape and the dimple particle position of the capsule during the motion. The results show that, for the one with strongest effect, it takes shortest time for the dimple particle to be back to its initial position. This suggests that with $0 < \alpha \leq 1$, we can model the behavior of the shape memory. Also with larger $\alpha$ value, we get stronger memory of the reference shape in the sense that membrane tank-treads back to the reference shape faster.
Figure 9: (Color online) Snapshots of the capsule in shear flow for $\alpha = 1$ (top two), 0.05 (middle two), and 0 (bottom two) with $C_a = 4.5467$ in a narrower channel. The time at which the motion of two walls is stopped are $t = 48.85$ ms, 47.6 ms, and 47.25 ms for $\alpha = 1$, 0.05, and 0, respectively.

3.2 Tumbling and tank-treading with a swinging mode

We have considered a capsule of the swelling ratio $s^* = 0.481$ with a fully non-uniform natural state ($\alpha = 1$) suspended in shear flow at the capillary numbers $C_a = 0.455, 9.093,$ and $90.934$ in a channel of the length $80\mu$m and width $20\mu$m. These capillary numbers give rise to two typical motions of the capsule, namely, (i) a tumbling motion and (ii) a tank-treading motion with a swinging mode, respectively. The inclination angle $\theta$ and the phase angle $\phi$ defined in Fig. 1(b) and Fig. 1(c), respectively, are used to described the capsule motion (see the Remark 3.1 for how to compute these two angles). Since the shape of capsule in shear flow is symmetric about its mass center and so is the reference angles in the bending term $E_b$, we can restrict the range of both inclination and phase angles to $[-90^\circ, 90^\circ]$. If the inclination angle has the local maxima and minima within $(-90^\circ, 90^\circ)$, the capsule is having a swinging mode; otherwise if the inclination angle decreases monotonously to $-90^\circ$ then jump to $90^\circ$, it has a tumbling motion. The criteria for the phase angle are the opposite. When the local maxima and minima of the phase angle are in $(-90^\circ, 90^\circ)$, the capsule has the tumbling motion. If the phase angle increases monotonously to $90^\circ$ and then jumps to $-90^\circ$, it means that the capsule is tank-treading.
At the capillary number $C_a = 90.934$, the capsule is elongated to an elliptical shape and performs a tank-treading motion with almost the same shape and inclination angle. When reducing the capillary number to 9.093, the capsule tank-treading with periodically oscillating inclination angle is obtained. We also observe that the shape of the capsule is deformed periodically. And at $C_a = 0.455$, the capsule keeps tumbling periodically with a small oscillation of the phase angle. These motions are illustrated by the snapshots and histories of the inclination and phase angles of the capsule in Figs. 10 and 11. During the tank-treading with a swinging mode, the capsule keeps changing its shape periodically with respect to the period of tank-treading. The shape deformation comes from the fact that during these motions the membrane tends to reduce the difference between the current bending angle $\theta_i$ and the reference angle $\theta_i^0$ to minimize the elastic energy. The obtained swinging mode is always coupled with the tank-treading motion. At the higher shear rate of $C_a = 90.934$, tank-treading motion is still accompanied by a swinging mode where the oscillation of inclination angle is very small (see Fig. 11). To demonstrate that the effect of the bending term $E_b$ given in Eqs. (2.5) and (2.9) is also a key factor (besides the viscosity ratio) on the capsule motion in shear flow, we have presented in Fig. 12 that the capsule at different nonuniform natural state undergoes either tank-treading motion or tumbling at a shear rate $500 \text{ s}^{-1}$. As the effect of the nonuniform natural state is weaker, the capsule just tank-treads; but under stronger effect, the capsule does tumble as shown in Fig. 12. We have also obtained that, for all choices of capillary numbers, the capsule with the uniform natural state undergoes tank-treading motion, which is same as in [22].

The inclination and phase angles in Fig. 13 do behave similarly to those in [12]. While the capsule is in swinging mode, the range of inclination angle decreases as the capillary number is increasing. Also a larger confinement ratio results in the speeding up of the rate of decreasing due to the presence of the wall closer to the capsule. On the other hand, while the capsule tumbles, the range of phase angle increases with the increasing of capillary number. but it does not show much dependence on the confinement ratio.
Figure 11: (Color online) Histories of the inclination angle (left) and the phase angle (right) at the capillary number $Ca = 0.455$ (top), 9.093 (middle), and 90.934 (bottom) associated with the tumbling (top) and tank-treading with swinging mode (middle and bottom), respectively.

The range of phase angle shows that the capsule tank-treads backward and forward while tumbling.

**Remark 3.1.** Concerning the calculation of the inclination angle and phase angle of a capsule shape, we assume the shape of capsule is symmetric with respect to its mass center. For the cases considered in this article, the capsule shapes are almost symmetric. Using the symmetry, we first find the longest distance between two membrane particles opposite to each other with respect to the mass center and then obtain the angle of the line segment connecting these two membrane particles with respect to the wall direction as the inclination angle of the capsule shape.

Concerning the phase angle, we first find two membrane particles whose distance is the shortest among all and use one of these two membrane particles as a reference particle to count how many springs there are between the first membrane particle and the reference membrane particle. Based on the number of springs, we then have the phase angle.
3.3 The intermittent behavior between tumbling and tank-treading

The intermittent behavior of capsule motion has been obtained in [12] due to the elastic energy term. Our computational results show that the bending energy density $E_b$ in Eqs. (2.5) and (2.9) does play a similar role and gives rise to the intermittent behavior of the capsule like those obtained in [12], a mixture of tumbling and TT with a swinging mode. When having the mixture of two motions, we notice that (i) while tumbling, the membrane does tank-tread backward and forward within a small range as presented in Fig. 13 and (ii) during tank-treading with a swinging mode, the inclination angle of the capsule only oscillates within a small range as in Fig. 13. An example of an intermittent behavior with a mixed dynamics of the capsule of the swelling ratio $s^* = 0.481$ obtained at $C_a = 4.410$ with $\alpha = 1$ is that the capsule performs one tumbling and one TT with a swinging mode in each cycle in a channel of the length $80 \mu m$ and width $20 \mu m$. Fig. 14 shows the snapshots of the capsule motion in one cycle as well as the histories of the inclination angle, the phase angle and the capsule energy. Since the capsule performs one tumbling and one TT with a swinging mode in each cycle, both angles show jumps (see the middle two of Fig. 14). From the snapshots of the capsule motion (the top one of Fig. 14), the marker “○” on the membrane moves in the clockwise direction at the first 4 different times while oscillating, then moves backward and forward, while tumbling, as shown at $t = 201.36 ms$, $201.6 ms$, and $201.76 ms$, and finally finishes one complete
Figure 13: (Color online) Phase angles while tumbling (left) and inclination angles while tank-treading (right) with respect to capillary numbers of the capsule of the swelling ratio $s^*=0.481$ at $\alpha=1$.

Figure 14: (Color online) Snapshots of the capsule shape and orientation in one cycle (top), histories of the inclination angle (middle left), the phase angle (middle right), and the energy over the unit thickness (bottom) of the capsule at $Ca=4.410$. Such motion shows a mixed dynamics of tumbling and one TT with a swinging mode in each cycle. The energy required for the tumbling in each cycle appears to be higher than that during the TT with a swinging mode, because
when the capsule oscillates, it has an elongated shape which is much closer to the original biconcave shape than those shapes when the capsule tumbles. Another typical example of the mixed dynamics of the capsule of the swelling ratio $s^* = 0.481$ with $\alpha = 1$ at $Ca = 4.4319$ is shown in Fig. 15. We have observed that the capsule has five tumbling and one TT with a swinging mode in each cycle (i.e., a periodic pattern of the mixed dynamics). In Fig. 15, the membrane moves backward and forward slightly during each tumbling; it finally moves across the hurdle and finishes a period of a tank-treading. Actually the intermittent region for the capsule of the swelling ratio $s^* = 0.481$ considered in section is about $4.274 < Ca < 4.456$ as $\alpha = 1$.

For the effect of the swelling ratio at $\alpha = 1$, we have tested the values of swelling ratio $s^* = 0.6, 0.7, 0.8$ and 0.9 and obtained that for the capsule of swelling ratio greater than 0.6, it is almost impossible to capture the intermittent region computationally since the size of the range of the capillary number for such region is about zero if it exists. The capsule of the swelling ratio $s^*$ can be characterized by its excess circumference $\Delta c = 2\pi(\frac{1}{\sqrt{s^*}} - 1)$.

For the biconcave shape of $s^* = 0.481$, its $\Delta c$ is 2.77638; but the one for an elliptical shape of $s^* = 0.9$ is 0.33987. The excess circumference $\Delta c$ is similar to the excess area used in [14]. For the small values of $\Delta c$, we do not expect to obtain the intermittent region. Our result is consistent with the results obtained by Tsubota et al. in [22] since the cells used in their simulations have the swelling ratio of 0.7.

4 Conclusions

In this paper, a computational model for the natural state of an inextensible capsule has been successfully combined with a spring model of the capsule membrane to simulate the motion of the capsule in simple shear flow. We have analyzed the dynamics of an inextensible capsule suspended in two-dimensional shear flow under the effect of the nonuniform natural state. Besides the viscosity ratio of the internal fluid and external
fluid of the capsule, the natural state effect also plays a role for having the transition between two well known motions, tumbling and tank-treading with the long axis oscillating about a fixed inclination angle, when varying the shear rate. Between tumbling and tank-treading, the intermittent behavior has been obtained for the capsule with a biconcave rest shape. The estimated critical value of the swelling ratio for having the intermittent transition behavior is less than 0.7. i.e., the capsules with the rest shape closer to a full disk do not have the intermittent behavior in shear flow. The intermittent dynamics of the capsule in the transition region is a mixture of tumbling and TT with a swinging mode. Just like the motion of TT with a swing mode, which can be viewed as a tank-treading with an incomplete tumbling, the membrane tank-treads backward and forward within a small range during the tumbling motion. The further study of the capsule dynamics and its intermittent behavior will be done in near future.

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References


