Onsager’s Variational Principle for the Dynamics of a Vesicle in a Poiseuille Flow

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Abstract – We propose a systematic formulation of the migration behaviors of a vesicle in a Poiseuille flow based on Onsager’s variational principle. Our model is described by a combination of the phase field theory for the vesicle and the hydrodynamics for the flow field. The time evolution equations for the phase field of the vesicle and the flow field are derived based on the Onsager’s principle, where the dissipation functional is composed of viscous dissipation of the flow field, bending energy of the vesicle and the friction between the vesicle and the flow field. We performed a series of simulations on 2-dimensional systems by changing the bending elasticity of the membrane, and observed 3 types of steady states, i.e. those with bullet, snaking, and slipper shapes. We show that the transitions among these steady states can be quantitatively explained with use of the Onsager’s principle, where the dissipation functional is dominated by the contribution from the friction between the vesicle and the flow field.

A migration of a bio-membrane in a narrow capillary is an important phenomenon for the understanding of the biological activities. For example, red blood cells are circulated in blood vessels. In such circulation, red blood cells show a large variety of shapes owing to their deformability. For example, in the experiment by Skalak et al. [1], a symmetric parachute and an asymmetric slipper shapes of the red blood cell were observed.

Recently, to elucidate the physical origin of the behaviors of red blood cells in a capillary, several simulation methods have been developed. Using surface element method, Noguchi et al. simulated the shape transition of a vesicle between an oblate shape and a prolate shape [2]. Kaoui et al. showed with use of the boundary integral method that the shape transition of a vesicle between the parachute and the slipper shapes is triggered by a decrease in the velocity difference between the vesicle center and the unperturbed external Poiseuille flow [3]. In these methods, the red blood cell is modeled as a closed surface which is discretized using triangular meshes.

Contrary to these studies, in the present work, we use field theories for both of the vesicle shapes and the flow field [4]. The use of the field theories is to avoid the difficulties in the above-mentioned discretized approaches using triangulation of the membrane surface, such as the treatment of the boundary condition between the vesicle surface and the external flow field. Moreover, using the field theories, we can evaluate the free energy of the vesicle quantitatively, which enables us to determine the equilibrium or steady states of the system. In the case of static simulations, the equilibrium shape of the vesicle is obtained by comparing the values of the total free energy of the vesicles among several candidates. Similarly to this free energy analysis in the static simulations, in the case of our dynamical simulations, stable steady states of the vesicle and the flow field are determined by comparing Onsager’s dissipation functional instead of the free energy of the system. In the following, we show the detail of our field theory based on Onsager’s principle and the simulation results for the shape deformations of a vesicle in a 2-dimensional Poiseuille flow.

Onsager’s principle is a fundamental framework that describes the complex non-equilibrium behaviors of soft materials, such as liquid crystals, gels, polymers and colloids [5][6]. Based on the Onsager’s principle, the dynamical equations for the vesicle and the flow field can be derived. In this study, we consider a two component system composed of the amphiphilic molecules that form the vesicle and a surrounding solvent.
First, we define the flow velocity \( \mathbf{v}(\mathbf{r}, t) \) as
\[
\mathbf{v}(\mathbf{r}, t) \equiv \phi_m(\mathbf{r}, t)\mathbf{v}_m(\mathbf{r}, t) + (1 - \phi_m(\mathbf{r}, t))\mathbf{v}_s(\mathbf{r}, t),
\]
where \( \mathbf{v}_m \) is the average velocity field of the amphiphilic molecules that form the membrane of the vesicle, \( \mathbf{v}_s \) is the velocity of the solvent, and \( \phi_m \) is the volume fraction of the amphiphilic molecules. Hereafter, unless explicitly stated, we will suppress the argument of time \( t \) for simplicity. As \( \phi_m \) is a conserved variable, the equation of continuity for \( \phi_m \) should be satisfied as
\[
\frac{\partial \phi_m(\mathbf{r})}{\partial t} = -\nabla \cdot (\phi_m(\mathbf{r})\mathbf{v}_m(\mathbf{r})).
\]
(2)

To obtain the equations of motion for \( \mathbf{v}, \mathbf{v}_m \) and \( \phi_m \), we introduce the Onsager’s dissipation functional \( R \) defined by
\[
R \equiv W_{\text{flow}} - \int p(\mathbf{r})\nabla \cdot \mathbf{v}(\mathbf{r}) d\mathbf{r} + \hat{F}_{\text{total}} + W_{\text{slip}},
\]
(3)
where we define
\[
W_{\text{flow}} \equiv \frac{1}{4} \int \eta(\mathbf{r}) \left[ \nabla \mathbf{v}(\mathbf{r}) + (\nabla \mathbf{v}(\mathbf{r}))^T \right]^2 d\mathbf{r},
\]
(4)
\[
W_{\text{slip}} \equiv \frac{1}{2} \int \frac{\phi_m(\mathbf{r})}{L(\mathbf{r})} (\mathbf{v}(\mathbf{r}) - \mathbf{v}_m(\mathbf{r}))^2 d\mathbf{r},
\]
(5)
and \( \eta(\mathbf{r}) \) is the viscosity of the flow, \( L(\mathbf{r}) \) is the mobility of the amphiphilic molecules and \( \hat{F}_{\text{total}} \) is the time derivative of the total free energy of the system which contains the bending energy of the vesicle shape and the Lagrange multipliers for the constraints on the total enclosed volume and the total surface area (detail will be shown later). The second term on the right-hand side of eq. (3) defines the Lagrange multiplier \( p(\mathbf{r}) \) for the incompressibility condition (\( \nabla \cdot \mathbf{v} = 0 \)), where \( p(\mathbf{r}) \) corresponds to the pressure. \( W_{\text{flow}} \) is the dissipation functional of the flow field and \( W_{\text{slip}} \) is the contribution from the friction between the vesicle and the flow field.

Due to the requirement of the non-equilibrium thermodynamics, the time developments of the vesicle shape and the flow field are given by minimizing the Onsager’s dissipation functional \( R \), which leads to the 2 conditions \( \delta R / \delta \mathbf{v}_m(\mathbf{r}) = 0 \) and \( \delta R / \delta \mathbf{v}(\mathbf{r}) = 0 \). Therefore, we obtain the following equations of motion for \( \mathbf{v} \) and \( \mathbf{v}_m \):
\[
\nabla \cdot [\eta(\mathbf{r})\nabla \mathbf{v}(\mathbf{r})] - \nabla p(\mathbf{r}) - \phi_m(\mathbf{r})\nabla \frac{\delta F_{\text{total}}}{\delta \phi_m} = 0,
\]
(6)
\[
\mathbf{v}_m(\mathbf{r}) = -L(\mathbf{r})\nabla \frac{\delta F_{\text{total}}}{\delta \phi_m} + \mathbf{v}(\mathbf{r}).
\]
(7)

Equation (6) represents the Navier-Stokes equation with Stokes approximation for a flow field with a low Reynolds number. The third term on the left-hand side of eq. (6) corresponds to the stress due to the bending energy of the vesicle. By combining eqs. (2) and (7), we obtain the time evolution equation for the vesicle shape as
\[
\frac{\partial \phi_m(\mathbf{r})}{\partial t} = \nabla \cdot \left( L(\mathbf{r})\phi_m \nabla \frac{\delta F_{\text{total}}}{\delta \phi_m} - \phi_m(\mathbf{r})\mathbf{v}(\mathbf{r}) \right),
\]
(8)
where the first term on the right-hand side of eq. (8) represents the Fick’s law of diffusion of the amphiphilic molecules, and the second term is the contribution from the advection due to the external flow field.

In order to simulate the vesicle behaviors based on eq. (5), we use phase field theory (PFT) \[4\,7\,9\]. In the PFT, the vesicle surface is represented by a scalar order parameter \( \psi \), which is called “phase field”. Inside and outside regions of the vesicle are specified by positive and negative values of \( \psi \). Therefore the vesicle surface is defined by \( \psi = 0 \). As such an interface is a topological defect of the field \( \psi \), the interface is stable and non-vanishing, which is an advantage of the PFT when simulating the flow behavior of the vesicle.

In the following, we rewrite eq. (8) in a form of a time evolution equation for the phase field \( \psi \). Similarly to the Ginzburg-Landau model for binary mixtures, the distribution of the amphiphilic molecules of the vesicle can be identified with \[3\,9\]
\[
\phi_m(\mathbf{r}) = \frac{1}{2} (1 - \psi(\mathbf{r})^2)^2 + \epsilon^2 |\nabla \psi(\mathbf{r})|^2,
\]
(9)
where \( \epsilon \) is the interface thickness. The mean curvature of the vesicle surface is obtained by a variation of the total surface area \( S (\propto \int \phi_m d\mathbf{r}) \) with respect to an infinitesimal displacement of the vesicle surface in its perpendicular direction. Therefore, we obtain the following formula
\[
H(\mathbf{r}) = -\psi(\mathbf{r}) + \psi(\mathbf{r})^3 - \epsilon^2 \nabla^2 \psi(\mathbf{r}),
\]
(10)
where \( H(\mathbf{r}) \) is a mean curvature multiplied by a constant that takes account of the dimensionality. With use of eqs. (9) and (10), eq. (8) is rewritten as
\[
\frac{\partial \phi_m(\mathbf{r})}{\partial t} = 2\epsilon^2 \nabla \cdot \left( \frac{\partial \psi(\mathbf{r})}{\partial \psi} \left| \nabla \psi(\mathbf{r}) \right| \right) + 2H(\mathbf{r}) \frac{\partial \psi(\mathbf{r})}{\partial t}.
\]
(11)

We first solve eq. (11) for a flat membrane with \( H = 0 \). Using the Green function of Coulomb potential generated by a point charge, we obtain 0-th order solution of eq. (11), i.e. a flat membrane solution, as follows:
\[
\left( \frac{\partial \psi(\mathbf{r})}{\partial t} \right)_0 = \frac{1}{2\epsilon^2} \nabla^2 \psi(\mathbf{r}) + \frac{1}{2\epsilon^2} \nabla^2 \psi(\mathbf{r})^2 \int G(\mathbf{r} - \mathbf{r}') \frac{\partial \phi_m(\mathbf{r}')}{\partial t} d\mathbf{r}',
\]
(12)
where \( G \) is Green function that takes the form \( G(\mathbf{r} - \mathbf{r}') = (1/4\pi)(\mathbf{r} - \mathbf{r}') /|\mathbf{r} - \mathbf{r}'|^3 \) in an infinite space. Substituting eq. (12) into the second term on the right-hand side of eq. (11) and repeating the same procedure that was done for the 0-th order solution, we obtain the time evolution equation for the phase field up to the first order in the mean curvature \( H \). (The resulting formula is not shown.)

As the simplest example of eq. (12), we first consider the case of no advection, i.e. the case where the second term on the right-hand side of eq. (5) is dropped. Using eqs. (8)-(11), we obtain the following equation of motion for \( \psi(\mathbf{r}) \):
\[
\left( \frac{\partial \psi(\mathbf{r})}{\partial t} \right)_0 = \nabla \cdot L(\mathbf{r})\phi_m \nabla \frac{\delta F_{\text{total}}}{\delta \phi_m}.
\]
\[ \frac{\partial \psi(r)}{\partial t} = -\frac{L(r)}{2\epsilon^2} \frac{\delta F_{\text{total}}}{\delta \psi(r)} + o(H^2), \] (13)

where \( o(H^2) \) means terms of order \( H^2 \) and higher orders. \( F_{\text{total}} \) is the total free energy of the membrane defined by

\[ F_{\text{total}} = \frac{\kappa}{2\epsilon^3} \int H(r)^2 \, dr + \sigma (S - S_0) + \gamma (V - V_0), \] (14)

where \( \kappa \) is the bending modulus of the vesicle, and \( \sigma \) and \( \gamma \) are Lagrange multipliers for the constraints on the total surface area \( S \) and on the total enclosed volume \( V \) that are fixed at the values \( S_0 \) and \( V_0 \), respectively. Equation (13) means that the conservation equation for \( \psi \) reduces to a non-conserved dynamical equation for \( \psi \) up to the leading order in the mean curvature \( H \).

Using eq. (13), the final form of the time evolution equation for \( \psi \) with the advection term is given by

\[ \frac{\partial \psi(r)}{\partial t} = -\frac{L(r)}{2\epsilon^2} \frac{\delta F_{\text{total}}}{\delta \psi(r)} - \frac{1}{2\epsilon^2} \frac{\nabla \psi(r)}{|\nabla \psi(r)|^2} \cdot \left\{ \phi_m(r) \mathbf{v}(r) \right\} + o(H^2). \] (15)

In an almost same procedure as that was used in the derivation of eq. (15), the functional derivative of the total free energy with respect to the membrane shape \( \delta F_{\text{total}}/\delta \phi_m \) is also obtained using \( \delta F_{\text{total}}/\delta \psi \), where \( \delta F_{\text{total}}/\delta \phi_m \) appears in the Navier-Stokes equation eq. (6) as the stress due to the bending energy of the membrane. For simplicity, hereafter, we assume that the system is 2-dimensional, and \( L(r) \) and \( \eta(r) \) are constant values \( L \) and \( \eta \). A 2-dimensional Poiseuille flow is realized by solving the Navier-Stokes equation eq. (6) with the conditions

\[ \mathbf{v}(x, 0) = \mathbf{v}(x, y_{\text{max}}) = 0, \] (16)

\[ \mathbf{v}(0, y) = \mathbf{v}(x_{\text{max}}, y), \] (17)

\[ \nabla \cdot \mathbf{v} = 0, \] (18)

where \( x \) and \( y \) are the coordinate in the directions parallel and perpendicular to the non-perturbed flow velocity, respectively. Equation (16) is the stick boundary condition at the boundary of the capillary at \( y = 0 \) and \( y = y_{\text{max}} \), and eq. (17) is the periodic boundary conditions at \( x = 0 \) and \( x = x_{\text{max}} \), respectively. Equation (18) means the incompressibility condition of the fluid.

Our model system is characterized by several non-dimensional parameters. In our 2-dimensional model, \( \nabla \) and \( S \) in eq. (14) represent the total enclosed area and the perimeter length of the vesicle, respectively. We define the vesicle size \( R_0 \) as the radius of a perfect circle that has the same perimeter length \( S \) of the vesicle. With use of the maximum velocity of the unperturbed Poiseuille flow \( V_{\text{max}} \), the bending modulus of the vesicle \( \kappa \) and the density of the solvent \( \rho \), we define the 3 non-dimensional parameters that characterize the system, i.e., the reduced volume \( v \), the Reynolds number \( \text{Re} \) and the capillary number \( \text{Ca} \) as

\[ \text{Re} = \frac{2\rho V_{\text{max}} R_0}{\eta}, \] (21)

\[ \text{Ca} = \frac{4\alpha V_{\text{max}} R_0^3}{y_{\text{max}} \left( \frac{1}{\text{Ca}} \right)_{0}}. \] (22)

In general, the flow field can be well described by the Navier-Stokes equation with the Stokes approximation for systems with low Reynolds number that satisfies \( \text{Re} < 0.1 \). This condition corresponds to a large value of \( \alpha \). In our simulations, we choose \( \alpha = 25 \) while changing \( V_{\text{max}} \), \( (1/\text{Ca})_0 \) and \( v \). This choice of \( \alpha \) validates the use of the Stokes approximation. In our simulations, we choose \( \alpha = 25 \) while changing \( V_{\text{max}} \), \( (1/\text{Ca})_0 \) and \( v \). This choice of \( \alpha \) validates the use of the Stokes approximation. In order to solve the phase field equation and the Navier-Stokes equation, we used a 2-dimensional mesh that has \( 128 \times 128 \) mesh points with a mesh width \( \Delta x = 0.5 \) and time step width \( \Delta t = 0.001 \).

In fig. 1 we show typical behaviors of the vesicle with \( v = 0.7 \) and \( V_{\text{max}} = 0.05 \). In this case, we found three steady states of the vesicle, i.e., a bullet shape, a slipper shape and a snapping oscillation. The bullet shape is a symmetric shape, where the vesicle shape is elongated in the flow direction (fig 1(a)). On the other hand, the slipper shape is an asymmetric shape, where the direction of the elongation axis of the vesicle is
Fig. 1: The time evolutions of the shapes of the vesicle with \( v = 0.7 \), \( V_{\text{max}} = 0.05 \), and \((1/Ca)_0\) equals to (a)1, (b)20 and (c)25, respectively. In steady states, (a) and (c) represent bullet and slipper shapes. We also observe a snaking oscillation in (b).

perpendicular to the flow velocity(fig.1(c)). These bullet and slipper shapes are known to be typical steady states of the vesicle in a Poiseuille flow \( \text{[2,3]} \). On the other hand, the snaking oscillation shown in fig.1(b) was rather recently discovered \( \text{[4]} \). In the snaking oscillation, the vesicle shape is elongated in a similar manner as the bullet shape. However, the rear end of the vesicle is temporarily bent just like the shape of a snake in its locomotion.

In fig.2, we show the lateral positions of the center of mass of the vesicle \( Y_0 \) in the vertical direction to the flow velocity. In these figures, \((1/Ca)_0\) is changed, while the maximum value of the flow velocity \( V_{\text{max}} \) is kept constant at the same value as was used in fig.1, i.e. \( V_{\text{max}} = 0.05 \). The left-hand side figure shows the lateral positions of the center of mass of the vesicle, where \((1/Ca)_0\) equals to 1, 20 and 25, respectively. When \((1/Ca)_0\) is increased, the stationary shape of the vesicle changes from (a) the bullet shape to (c) the slipper shape. The snaking behavior is found for (b) the intermediate value. In the right-hand side figure of fig.2 we show the temporal behaviors of the lateral positions of the center of mass of the vesicle for the snaking behavior. With increasing \((1/Ca)_0\), which corresponds to increasing the bending modulus \( \kappa \), the amplitude of the oscillation of the lateral position is increased, which means that the stress of the flow field induced by the bending elasticity of the vesicle is important for the snaking behaviors.

To explain such transitions among different steady states of the vesicle quantitatively, we focus on the dissipation functional defined by eqs.\( \text{[3-5]} \). In steady states, contribution from the time derivative of the total free energy \( \dot{F} \) is vanishing. (In the case of the snaking motions, time average of \( \dot{F}_{\text{total}} \) is zero instead of the instantaneous value of \( \dot{F}_{\text{total}} \).) Moreover, we found that the second terms on the right-hand side of eq.\( \text{[3]} \) is negligible due to the incompressible conditions of the flow field. Figure 3 shows the dependences of the components of the dissipation functional (for simplicity, we call this just dissipation in the following) on \((1/Ca)_0\), where the value of \((1/Ca)_0\) is a measure of the importance of the bending elasticity of the vesicle compared with that of the fluid.

Figure 3(a) shows the contributions from the fluid flows in the outside and inside regions of the vesicle. These values represent the deviations in the dissipation from that in the unperturbed Poiseuille flow. When the value of \((1/Ca)_0\) is increased, bullet, snaking and slipper shapes appear in this order. At each transition point between different shapes, we observe a kink in the curve, which indicates an occurrence of a transition from one stable branch to another. This is a sign of a 1st order phase transition.

In the bullet region ((1/Ca)_0 < 5), the dissipation of the outside fluid is increasing as (1/Ca)_0 is increased while the change in the dissipation of the inside fluid is less pronounced. The extra dissipation of the outside fluid from the unperturbed Poiseuille flow is due to the disturbance near the surface of the vesicle, which plays the role of an essentially stick boundary for the fluid. When (1/Ca)_0 is small (a flexible vesicle), the vesicle shape is deformed by the fluid flow so that the dissipation of the flow is minimized. Such an adjustment of the vesicle shape becomes less effective when (1/Ca)_0 becomes large because of the increasing stiffness of the vesicle. This leads to an increase in the dissipation of the outside fluid. On the other hand, the inside fluid is static in the frame of the enclosing vesicle because the bullet shape does not change its shape with no flow on the membrane just like a rigid container for the inside fluid. In fig.3(b)(ii), the sum of the contributions from the inside and outside fluids is shown. According to the above discussion, the slight increase of this sum in the bullet region is coming from the outside fluid. On the other hand, fig.3(b)(iii) shows the dissipation due to the friction associated with the slip motion between the membrane and the fluid (both inside and outside of the vesicle) along the vesicle surface. One can observe that the increase of (1/Ca)_0 induces an increase of the dissipation.
motion (fig.3(b)(iii)) induced by the tank-treading motion. Reduction in the slope of the dissipation due to the slip motion overcomes the increase in fig.3(b)(ii) in the amount as that of the outside fluid. The sum of these two contributions gives the increase in fig.3(b)(ii) in the amount as that of the outside fluid. The sum of these dissipation of the inside fluid, which is almost the same justment is realized at the sacrifice of the increase in the adjustment is realized at the sacrifice of the increase in the dissipation due to the slip motion (fig.3(b)(iii)). Such a decrease in the dissipation due to the slip motion (fig.3(b)(iii)). Such a decrease in the dissipation due to the slip motion overcomes the increase in the dissipation due to the fluid(fig.3(b)(ii)), and the total dissipation $R$ (fig.3(b)(i)) has a smaller slope than that in the bullet region. The difference in the slopes of the total dissipation between bullet and snaking regions leads to a transition from the bullet branch to the snaking branch at around $(1/Ca)_0 \sim 5$.

For the slipper region($25 < (1/Ca)_0$), the effect of the tank-treading motion is much more pronounced, which is indicated by the abrupt decrease in the dissipation due to the slip motion (fig.3(b)(iii)). Such a decrease in the dissipation due to the slip motion overcomes the increase in the dissipation due to the fluid(fig.3(b)(ii)), and the total dissipation $R$ (fig.3(b)(i)) has a smaller slope than that in the snaking region. This is again the origin of the second transition from the snake shape to the slipper shape at around $(1/Ca)_0 \sim 22$.

In fig.4 we show the phase diagram of the behaviors of the vesicles with $(1/Ca)_0 = 25$. The horizontal and the vertical axes represent $V_{\text{max}}$ and $\nu$, respectively. When the reduced volume $\nu$ becomes larger, the vesicle changes its shape from an asymmetric shape(slipper) to a symmetric shape(bullet). Although this symmetric-asymmetric transition is qualitatively similar to that reported in preceding researches [3, 10, 11], there is a certain difference between our results and the results reported by Kaoui et al. [10]. In order to explain this difference, let us focus on the steady shapes of the vesicle in the case $\nu = 0.6$, for which we obtain only slipper shapes as is shown in fig.4. In this case, the capillary number Ca and the measure of the confinement of the vesicle inside the capillary $2R_0/y_{\text{max}}$ take the values Ca $> 4.5$ and $2R_0/y_{\text{max}} \simeq 0.44$, respectively. For the same conditions, however, Kaoui et al. showed that the slipper shape and the parachute shape are the steady shapes instead of the slipper shape we obtained [11].

In the snaking region($10 < (1/Ca)_0 < 20$), the slope of the curve for the outside fluid (left-side figure of fig.4(a)) is smaller than that in the bullet region. This behavior means that the perturbation to the outside fluid imposed by the vesicle is more relaxed for the snake shape than the bullet shape. As there is a tank-treading motion of the membrane for the snake shape as well as the change in its whole shape, it is easier for the snaking vesicle to adjust itself to the outside fluid than the bullet shape so that the friction of the outside fluid is reduced. This adjustment is realized at the sacrifice of the increase in the dissipation of the inside fluid, which is almost the same amount as that of the outside fluid. The sum of these two contributions gives the increase in fig.3(b)(ii) in the snaking region, which has a slightly larger slope than that in the bullet region. This increase is compensated by the reduction in the slope of the dissipation due to the slip motion (fig.3(b)(iii)) induced by the tank-treading motion of the vesicle surface. As a result, the total dissipation $R$ (fig.3(b)(ii)) has a smaller slope than that in the bullet region. The difference in the slopes of the total dissipation between bullet and snaking regions leads to a transition from the bullet branch to the snaking branch at around $(1/Ca)_0 \sim 5$.

Fig. 4: Phase diagram of the behaviors of the vesicle with $(1/Ca)_0 = 25$. Horizontal and vertical axes mean $V_{\text{max}}$ and $\nu$. Each symbol represents the simulated point. Blue symbol represents the slipper shape, orange one the bullets shape, red one the zigzag motion and the green one the snaking motion, respectively. The stationary slipper and bullet shapes are shown besides the symbols. The boundaries are guide to the eyes.
reason for this difference between our result and their result is the dissipation due to the slip velocity \( W_{\text{slip}} \), which is included only in our model. By combining eqs. (5) and (7), we obtain the relation

\[
W_{\text{slip}} = -\frac{1}{Ca_0} \int_0^\phi \left[ \frac{1}{2} \nabla \delta F_{\text{total}} / \delta \phi_m \right]^2 d\phi,
\]

where \( |\nabla (\delta F_{\text{total}} / \delta \phi_m)| \) corresponds to the diffusion flux of the amphiphilic molecules on the vesicle surface that reduces the total free energy of the vesicle \( F_{\text{total}} \). Such a diffusion leads to a difference in the velocities between the amphiphilic molecules and the external flow field, which is the reason why the vesicle with a large deformation is not preferable with respect to \( W_{\text{slip}} \). Generally speaking, the slipper-shaped vesicle shows a smaller deformation than the parachute-shaped vesicle, because the amphiphilic molecules on the slipper-shaped vesicle undergo a tank-treading motion, which prevents large deformation of the vesicle due to the shear force of the external flow. As a result, the slipper shape is selected as the stable state.

In Fig. 5, we found two types of (damping) oscillations of the vesicle motions, i.e., snaking and zig-zag motions, which can be observed in the region between the stable regions of the slipper and bullet shapes. The zig-zag motion is a damping oscillation in which the vesicle takes the parachute and the slipper shapes alternatively as is shown in Fig. 5. The vesicle moves toward the wall of the capillary with the slipper shape and then turns. The parachute shape appears at this turning point. After such a turning, the vesicle moves toward the other wall again with the slipper shape. It is difficult to obtain the final stationary shape of the vesicle in this case because the period of the damping oscillation is very long. Therefore, we cannot identify which shape is chosen as the stationary shape in the region of zig-zag oscillations in Fig. 5.

So far, we have shown two types of oscillations, i.e., the snaking motion and the zig-zag motion. In addition to these long-lived oscillations, we have also found (damping) a vacillating-breathing oscillation [12] in the region \( \nu < 0.65 \). All of these oscillations have already been reported in preceding works, where the vesicle is modeled with discretized meshes [13,14]. In these works, the vesicle deformations are induced by two different forces, i.e., the force due to the flow field and that due to the bending elasticity of the vesicle, both of which are also taken into account in our simulations in the diffusion of the amphiphilic molecules. On the other hand, Kaoui et al. proposed another model where the vesicle deforms due to the flow field without any slips. [10] In this case, they reported only snaking oscillations and they did not observe the zig-zag and the vacillating-breathing oscillations. This result means that the slip velocity of the vesicle is important in realizing the various temporal oscillations.

In conclusion, by using a combination of the PFT and Navier-Stokes equation, we derived, up to the first order of the local mean curvature of the vesicle, a set of dynamical equations which are equivalent to those obtained using the Onsager’s principle. Using this model, we performed dynamical simulations of the vesicle in a 2-dimensional Poiseuille flow which is a model of a red blood cell in a blood vessel. We simulated this model and found four types of behaviors of the vesicle, such as bullet shape, slipper shape, snaking motion and zig-zag motion. An analysis based on the Onsager’s dissipation functional revealed that the origin of these behaviors is the slip between the velocities of the vesicle and the flow field.

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