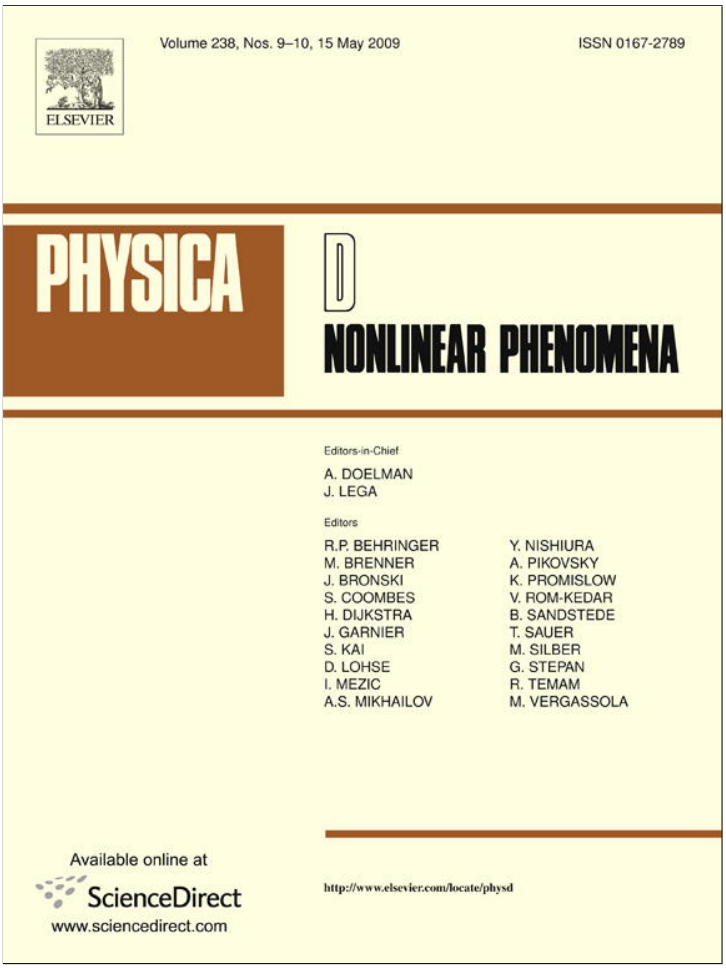

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Energetic variational approaches in modeling vesicle and fluid interactions☆

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ABSTRACT

In this paper, we establish a hydrodynamic system to study vesicle deformations under external flow fields. The system is in the Eulerian formulation, involving the coupling of the incompressible flow system and a phase field equation. The phase field mixing energy can be viewed as a *physical* approximation/regularization of the Helfrich energy for an elastic membrane. We derive a self-consistent system of equations describing the dynamic evolution of vesicles immersed in an incompressible, Newtonian fluid, using an energetic variational approach. Numerical simulations of the membrane deformations in flow fields can be conducted based on the developed model.

1. Overview

The study of formation and dynamics of vesicle membranes has been an active source of experimental and theoretical investigations in interface sciences for the past several decades. Vesicle shapes exhibit a rich set of geometric structures in various mechanical, physical and biological environments. The study of the morphological changes of vesicles presents interesting challenges to the efficient and accurate numerical simulations, effective mathematical modeling and rigorous analysis. The variety of equilibrium shapes assumed by vesicles in biological experiments, such as spheres, discocytes, stomatocytes, tori and double tori are concrete examples of minimizers of different surface energies, such as the bending elasticity (Willmore, mean curvature square) energy in the calculus of variations and its different variations [1] like the general Helfrich energy [2,3]. However, in studying features of vesicles such as the deformation of blood cells in capillaries or exocytosis processes, one must additionally understand the coupling of these configurations with the background fluid momentum [4–14], as well as other external fields, e.g. electric fields. This paper addresses this issue in the modeling and simulation of the deformation of simple vesicles coupled with incompressible flow fields by developing an energetic variation based diffuse interface approach.

1.1. Modeling of the vesicle structure

Let $\Sigma \subset \mathbb{R}^3$ be a smooth, compact surface without boundary representing the membrane of the vesicle. The quasi-static deformation and equilibrium configuration of a vesicle is mainly characterized by its interfacial energy [15,1]:

$$\mathscr{H}(\Sigma) = \kappa_0 \int_\Sigma \frac{1}{2}(H(x) - \kappa(x))^2 \mathrm{d}S(x) + \overline{\kappa} \int_\Sigma K(x)\mathrm{d}S(x). \qquad (1.1)$$

Often, $\mathscr{H}(\Sigma)$ is called the Helfrich bending elasticity energy of the surface Σ. Here

$$H(x) = \frac{1}{2}(k_1(x) + k_2(x)), \qquad K(x) = k_1(x) \cdot k_2(x)$$

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where $k_1(x)$ and $k_2(x)$ are the principle curvatures at a point $x \in \Sigma$. κ_0 and $\overline{\kappa}$ are two bending rigidities and $\kappa(x)$ denotes the spontaneous curvature at a point $x \in \Sigma$ which arises due to inhomogeneities in the bilayer lipid membrane structure. Due to the classic Gauss–Bonnet formula, for smooth surface Σ, the last integral in (1.1) is $2\pi\overline{\kappa}\chi(\Sigma)$ where $\chi(\Sigma)$ is the Euler characteristic of the surface. It encodes the topology of the lipid membrane: if g is the genus of the surface, then $\chi(\Sigma) = 2 - 2g$. If the evolution of the vesicle membrane does not change its topology, then $\chi(\Sigma)$ is constant and the second integral in (1.1) can be viewed as a constant added to the simplified energy

$$\mathscr{H}_0(\Sigma) = \kappa_0 \int_\Sigma \frac{1}{2}(H(x) - \kappa(x))^2 \mathrm{d}S(x). \tag{1.2}$$

For simplicity of exposition, the phase field model put forth in what follows is based on (1.2). However, the phase field vesicle deformation model (Section 2.1) can also be modified to model the full Helfrich energy (1.1) by adding an approximation of the Euler characteristic as defined in [16].

Canham [2] and Helfrich [3] were among the first to formulate the conformational shapes of vesicles in terms of the energy $\mathscr{H}_0$ on the basis that the bending energy of the vesicle should depend on the symmetric, quadratic terms of k_1 and k_2 in the Taylor expansion of a curvature dependent Lagrangian energy functional.

In this paper, we are interested in modeling the interaction of a vesicle with the fluid field. Physical considerations lead us to choose a total surface area and a enclosed volume for the vesicle which are fixed in time: the constant surface area is a consequence of the incompressibility of the membrane, while the constant volume is based on the consideration that, for a fluctuating vesicle with the inside pressure and outside pressure balanced by the osmotic pressure, the change in volume is normally a much slower process in comparison with the shape change. These two constraints are widely used in the biophysical studies of vesicles [1].

We note that there are also experimental studies on the membrane area compressibility, as well as the thickness compressibility (see [17,18]). Moreover, there are other variations and additions to the volume and surface area constraints, for example, in [19], a bilayer-coupled model is proposed based on the bilayer-couple hypothesis. Assuming that the area per lipid molecule is fixed and there is no molecular exchange between the inner and outer leaves, this model leads to a constraint on the area difference

$$\Delta A = \kappa_1 \int_\Sigma H(x)\mathrm{d}S(x).$$

There are also recent works on enforcing membrane local incompressibility constraints [20]. Note that at this point, we do not incorporate a constant differential area constraint but the formal asymptotics in Section 4 indicate that local incompressibility of the membrane is a feature of our phase field model.

Let $n = n(x)$ be the outward pointing unit normal to Σ at the point $x \in \Sigma$. The surface gradient and surface divergence are defined respectively by:

$$\nabla_\Sigma u = (I - n \otimes n)\nabla, \quad \text{and} \quad \mathrm{div}_\Sigma = \mathrm{tr}\,\nabla_\Sigma.$$

The surface Laplacian is given by

$$\Delta_\Sigma = \mathrm{tr}\,\nabla_\Sigma\nabla_\Sigma = \Delta - 2Hn\cdot\nabla - n\otimes n : \nabla^2.$$

The mean curvature may be defined as follows;

$$H = -\frac{1}{2}\nabla_\Sigma \cdot n = -\frac{1}{2}\nabla\cdot n, \tag{1.3}$$

the last equation making sense if n is defined by $n = \nabla\rho/|\nabla\rho|$ for some scalar valued function ρ with $\rho|_\Sigma \equiv 0, \nabla\rho|_\Sigma \neq 0$ for example. In case ∇n is symmetric, we have a second important identity:

$$4H^2 - 2K = \mathrm{tr}((\nabla n)^2). \tag{1.4}$$

A vesicle which moves with the fluid generally deforms under the flow field, thereby changing the Helfrich energy $\mathscr{H}_0(\Sigma)$. If the membrane is not in the steady state, it exhibits an instantaneous force composed of an elastic force, surface tension due to the surface area constraint and a pressure due to the volume constraint. The elastic force is composed of the normal force

$$\left(\Delta_\Sigma(H-\kappa) + 2(H-\kappa)(H^2 - K + H\kappa)\right)n, \tag{1.5}$$

surface tension μHn and pressure λn for some Lagrange multipliers μ and λ stemming from the surface area and volume constraints. A derivation of (1.5) from perturbations of Σ by arbitrary vector fields can be found in [21] while the classical case for normal vector fields can be found in [22]. The absence of a traction in (1.5) can be explained by the invariance of the Helfrich energy, surface area and volume under tangential deformations of Σ.

1.2. Energetic variational approach

Incorporating (1.5) along with the surface $\Sigma \subset \mathbb{R}^3$ into a conventional, workable numerical model is in general non-trivial. In order for (1.5) to be continuously defined, the surface must be at least four times differentiable. In the presence of singularities, such as the formation of necks during coalescence or pinching from extension, (1.5) is not well defined and in practice must be replaced by other auxiliary/regularized forces. The deformation may be sensitive to the choice of the auxiliary force and in turn may not be physical. In these cases, it is more appropriate to return to the weak formulation of (1.5) in terms of the flow in the energy landscape of $\mathscr{H}_0$.

The energy of a vesicle with fluids both inside and outside is composed of the kinetic energy of the fluid and $\mathscr{H}_0$ (assuming the density of the membrane is comparable to the fluid). The fluid will deform, transporting the vesicle, in such a way as to transfer the total exchange of kinetic energy to the Helfrich energy of the vesicle membrane, and vice verse. The basic physical law behind such exchange of energies is the least action principle (LAP) or principle of virtual work (PVW). The strategy we propose in this paper is to approximate the Helfrich energy (1.2) by a phase field functional (2.1) corresponding to a diffuse interface description of the vesicle, and to define an action (2.14) in terms of the phase field energy and then derive evolution equations which result from the variation of the action functional. This method is consistent with the general framework of the energetic variational approach (EVA) developed for complex fluids with underlying microstructures or patterns [23].

The key difficulty in studying the dynamics of the fluid–structure interaction is the fact that the natural description for elasticity is in Lagrangian coordinate (Hooke's law) and for fluids, in Eulerian coordinates. The Helfrich-type surface energy functionals are in Lagrangian coordinate as well. The introduction of the phase field (labeling) function provides an analytical description for geometric motions in Eulerian coordinates. The art within this framework is the realization/approximation of various surface energy in terms of this phase function.

The phase field energetic variational approach has many advantages. The most notable one is that the model equations are defined in observer's (Eulerian) coordinates. This highly simplifies the numerical approximation because it suffices to consider a fixed computational grid rather than tracking the position of the interface. A corollary of this formulation is that the phase field is insensitive to topological changes of its level sets which readily

undergo shape transitions. The third advantage is that the fourth order phase field equations are defined in weak form. Consequently, conventional mixed and discontinuous Galerkin finite elements, along with the spectral methods, may be used to discretize the equations. Finally, the energetic variational approach guarantees the consistency of exchange between different parts of energy functionals. We derive the canonical energy law (2.18) associated with the variational approach. It states that the total sum of the kinetic and phase field energy are dissipated due to viscous losses and other regularization/relaxations rates. In the next section we define the phase field approximation of the Helfrich energy, the action functional and derive the evolution equations from the action functional via the least action principle (LAP).

The idea of the phase field approach goes back to [24] and it has been extensively studied [25–30]. A labeling function (usually referred to as a phase field) is introduced on the computational (physical) domain. The membrane is approximated/regularized by the transition region of the phase field. The inside/outside of the vesicle is represented by the pre-image of $\mathbb{R}_+$ and $\mathbb{R}_-$ respectively under the phase field function.

In previous works, the authors have established phase field representations of the Helfrich energy both with and without spontaneous curvature, together with the corresponding topological quantities such as the Euler number. In [31,46], we studied a phase field representation of the Helfrich energy (2.1) when the spontaneous curvature is zero, with the constraints of the membrane surface area and enclosed volume. We numerically studied the equilibrium configuration of local minimizers and probed the bifurcation landscape of vesicle configurations by varying area and volume. In [33], we included the spontaneous curvature effect in the simulations. In these works we were able to recover many of the experimentally observed vesicle shapes/configurations/patterns, such as those reported in [34]. Formal asymptotic analysis of the convergence of the phase field model (to the original sharp interface model as the transition width of the diffuse interface approaches zero) were performed in [35,36]. In [32] and later in [16], we derived numerical methods to approximate the integral of the Gauss curvature with an aim at obtaining (or controlling) topological information in phase field simulations. The schemes are based on the Gauss–Bonnet formula, giving not only a better indicator of topological changes than the energy functional, but in fact, quantized jumps when the computed surface passed singularities. A similar hydrodynamic phase field model has also been given in [7], with the main distinct feature being the assumption on the local area preservation, while our model assumes the global area preservation. In another recent work [20], a thermodynamic phase field model has been studied for vesicles under the assumption of local membrane incompressibility. The phase field energy for the vesicle is based on the formulation of the surface tension energy instead of the elastic bending energy. The rigorous study of the sharp interface limit of the dynamic models in [7,20] still remains to be carried out.

2. The phase field vesicle deformation model

We approximate the deformation of the fluid bound vesicle by means of an incompressible flow and phase field coupling. We adopt the phase field approximation of the Helfrich energy, as well as approximations of the vesicle surface area and volume as in [31]. The corresponding body forces which appear in the momentum equation are derived from these energies through the least action principle.

Motivated by the theory of phase transitions we pose the following phase field approximation of the Helfrich energy. Let $\Omega \subset \mathbb{R}^3$ be the computational domain. For a sufficiently smooth function ϕ (called the phase field), we define

$$\mathscr{G}_\epsilon(\phi) := \frac{1}{c_0}\int_\Omega \frac{\epsilon}{2}\left(\Delta\phi(x) - \frac{(\phi^2(x)-1)\phi(x)}{\epsilon^2} - \frac{2\kappa(x)(\phi^2(x)-1)}{\epsilon}\right)^2 \mathrm{d}x. \tag{2.1}$$

The order of thickness of the phase transition region is characterized by the small, positive parameter ϵ, $\kappa(x)$ is defined by a suitable extension of the spontaneous curvature over Ω and c_0 is a normalization constant which would ideally guarantee that $\mathscr{G}_\epsilon(\phi)$ converges to $\mathscr{H}_0(\Sigma)$ as ϵ converges to 0. In the remainder of this paper we will interchangeably refer to both $\mathscr{H}_0$ and its approximating functional $\mathscr{G}_\epsilon$ as the Helfrich energy when the context is clear. We note that (2.1) is one variant of a phase field energy functional posed by De Giorgi in [37] which has recently gained interest in the phase transition community as well as in image processing and applications [38]. The Γ-limit of a related functional to $\mathscr{H}_0$ has been studied recently in [39–41].

The vesicle surface area and volume are approximated by

$$\mathscr{S}_\epsilon(\phi) := \frac{1}{c_1}\int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{(\phi^2-1)^2}{4\epsilon}\,\mathrm{d}x,$$

$$\text{and}\quad \mathscr{V}(\phi) := \int_\Omega \phi\,\mathrm{d}x$$

respectively. Again c_1 is chosen so that $\mathscr{S}_\epsilon(\phi)(\phi)$ converges to the surface area of Σ as ϵ converges to zero. In this paper, we use the prime ($'$) notation to denote the Euler–Lagrange operator, i.e.

$$\int_\Omega \mathscr{E}'(\phi)v\,\mathrm{d}x = \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(\phi + tv)|_{t=0},$$

for $v \in C_0^\infty(\Omega)$ and a suitably differentiable functional $\mathscr{E}$.

Note that (2.1) is a simplified form of the general Helfrich energy $\mathscr{H}_0(\Sigma)$ in (1.1), with the contribution from the Gaussian curvature or the topological term neglected. In [32], we developed a series of phase field formulations to approximate the topological term which may be potentially incorporated into (2.1) to give a full treatment of (1.1). We leave such considerations to future works. The current work remains valid for vesicle evolutions without any change in the total Gaussian curvature contribution (see, for example, the simulation given in Section 3).

2.1. Evolution equations

The phase field and incompressible flow coupling is

$$u_t + u\cdot\nabla u + \nabla p = \nu\Delta u + \left(\mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi)\right)\nabla\phi, \tag{2.2}$$

$$\nabla\cdot u = 0, \tag{2.3}$$

$$\phi_t + u\cdot\nabla\phi = -\gamma\left(\mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi)\right), \tag{2.4}$$

$$\mathscr{S}_\epsilon(\phi) = \mathscr{S}_\epsilon(\phi_0); \qquad \mathscr{V}(\phi) = \mathscr{V}(\phi_0) \tag{2.5}$$

in Ω with the initial condition

$$u(\cdot,0) = u_0, \qquad \phi(\cdot,0) = \phi_0, \tag{2.6}$$

and the boundary condition

$$u|_{\partial\Omega} = 0, \qquad \phi(\cdot,t)|_{\partial\Omega} = 1. \tag{2.7}$$

Eqs. (2.2) and (2.3) are the Navier–Stokes equations of a viscous fluid with unit density and with a force defined in terms of ϕ. Eq. (2.3) is the condition of incompressibility. We use $u(x,t)$ as the velocity field of the fluid, p the pressure and ϕ the phase field which marks the position of the vesicle. We assume that ν, the fluid viscosity, is a positive constant throughout both fluid phases and the interface.

Eq. (2.4) is a relaxed transport equation of ϕ with advection by the velocity field u. We have added a regularization term on the right-hand side. The regularization parameter γ is a small, positive constant. The regularization term can also take on other forms which are all chosen to ensure the consistent dissipation of energy.

The unknown parameters $\lambda(t)$ and $\mu(t)$ are Lagrange multipliers associated with the constraints (2.5). To understand how these are determined, we multiply Eq. (2.4) by unity and $\mathscr{S}'_\epsilon(\phi)$ respectively and integrate over Ω. We find then that $\lambda(t)$ and $\mu(t)$ implicitly solve the linear system of equations:

$$\lambda(t)|\Omega| + \mu(t)\int_\Omega \mathscr{S}'_\epsilon(\phi)\,dx = -\int_\Omega \mathscr{G}'_\epsilon(\phi)\,dx$$

$$\lambda(t)\int_\Omega \mathscr{S}'_\epsilon(\phi) + \mu(t)\int_\Omega (\mathscr{S}'_\epsilon(\phi))^2\,dx = \int_\Omega \left(\gamma^{-1}u\cdot\nabla\phi - \mathscr{G}'_\epsilon(\phi)\right)\mathscr{S}'_\epsilon(\phi)\,dx.$$

This system is solvable since the determinant of coefficients on the left-hand side of the system is

$$|\Omega|\left(\int_\Omega (\mathscr{S}'_\epsilon(\phi))^2\,dx\right)^{1/2} - \left(\int_\Omega \mathscr{S}'_\epsilon(\phi)\,dx\right)^2 > 0$$

provided $\mathscr{S}'_\epsilon(\phi)$ is not a constant function. Else, only one independent Lagrange multiplier is required which can be determined from Eq. (2.2).

2.2. Principle of virtual work

The motivation for Eqs. (2.2) and (2.3) comes from the PVW (or LAP). This principle states that the fluid deforms in such a way as to extremize the total exchange of kinetic energy to the internal energy. In our case, the internal energy is the bending energy associated with vesicle interface, namely $\mathscr{G}_\epsilon(\phi)$. In order to derive the force balance equation, we postulate an action functional, apply the PVW by extremizing the action functional with respect to admissible fluid deformations and define the thermodynamically consistent regularization.

Let Ω be a bounded, closed subset of $\mathbb{R}^3$ with piecewise smooth boundary. Points in Ω are denoted by p and $t \in [0,T]$ denotes time. A motion of the region Ω is a one-parameter family of deformations $\mathsf{x} : \Omega\times[0,T]\to\Omega$ with the property that x is a smooth function of p and t, $\mathsf{x}(\cdot,0) = \mathrm{id}_\Omega$ and $\det(\nabla_p\mathsf{x}(\cdot,t)) > 0$ for each t. Motivated by the no-slip boundary condition in (2.7), we say x fixes the boundary of Ω if $\mathsf{x}(p,t) = p$ whenever $p\in\partial\Omega$. For fixed t, $\mathsf{x}(\cdot,t)$ is a diffeomorphism. For $p\in\Omega$, the path line of a particle which initially lies at p is $\{\mathsf{x}(p,t) : t\in[0,T]\}$.

Associated with a motion x is the smooth velocity field $u : \Omega\times[0,T]\to\mathbb{R}^3$ defined by

$$u(\mathsf{x}(p,t)) = \frac{d}{dt}\mathsf{x}(p,t). \tag{2.8}$$

The velocity field u vanishes on $\partial\Omega$ if x fixes the boundary of Ω. If x^s is a smooth, one-parameter family of motions which fix the boundary of Ω, then one has a velocity field $v : \Omega\times[0,T]\to\mathbb{R}^3$ defined by

$$v(p,t) = \left.\frac{d}{ds}\mathsf{x}^s(p,t)\right|_{s=0}. \tag{2.9}$$

The Eulerian velocity field v^* associated with v is defined by $v^*(\mathsf{x}(p,t),t) = v(p,t)$. Similarly for u, the velocity fields v and v^* vanish on $\partial\Omega$.

We will use motions to define various transformations of scalar valued functions on Ω and study the effect of these transformations on functionals. Given a function $\phi_0 : \Omega\to\mathbb{R}$ we define functions $\phi, \phi^s : \Omega\times[0,T]\to\mathbb{R}$ which take the constant value $\phi_0(p)$ along path lines of a particle initially lying at p under the motions x and x^s respectively;

$$\phi(\mathsf{x}(p,t),t) = \phi^s(\mathsf{x}^s(p,t),t) = \phi_0(p). \tag{2.10}$$

Note that ϕ and ϕ^s are well defined because $\mathsf{x}(\cdot,t)$ and $\mathsf{x}^s(\cdot,t)$ are one-to-one and onto Ω for each t. We call ϕ a labeling function because a particle initially lying at a point p retains the initial label $\phi_0(p)$ in time. By the chain rule, (2.10) is equivalent (assuming ϕ_0 is regular) to the labeling functions ϕ and ϕ^s satisfying the transport equations

$$\frac{\partial\phi}{\partial t} + u\cdot\nabla\phi = 0, \qquad \phi(\cdot,0) = \phi_0, \tag{2.11}$$

$$\left.\frac{\partial\phi^s}{\partial s}\right|_{s=0} + v^*\cdot\nabla\phi^0 = 0, \qquad \phi^0(\cdot,0) = \phi_0. \tag{2.12}$$

If $\mathscr{E}$ is a differentiable functional defined for ϕ^s, then by definition of the Euler–Lagrange operator $\mathscr{E}'(\cdot)$ and the fact that $v^*\cdot\nabla\phi \in C_0^\infty(\Omega)$,

$$\left.\frac{d}{ds}\mathscr{E}(\phi^s)\right|_{s=0} = -\int_\Omega \mathscr{E}'(\phi)v^*\cdot\nabla\phi^0\,dx. \tag{2.13}$$

Given a motion x which fixes the boundary of Ω, define the action

$$\mathscr{A}(\mathsf{x}) = \int_0^T\int_\Omega \frac{1}{2}|\mathsf{x}_t|^2\,dp - \mathscr{G}_\epsilon(\phi)\,dt. \tag{2.14}$$

The fluid occupying the region Ω is assumed to be incompressible and the subregion bounded by the vesicle is assumed to have constant volume and surface area in time. Thus we will restrict our attention to motions x which are volume preserving and for which $\mathscr{S}_\epsilon(\phi(\cdot,t))$ is constant with respect to t where ϕ is the labeling function defined by (2.10) with initial label ϕ_0 from (2.6). Volume preserving motions automatically satisfy the volume constraint of the vesicle, $\mathscr{V}(\phi) = \mathscr{V}(\phi_0)$ in (2.5), because of the change of variables formula. This set of admissible motions is

$$\mathfrak{X} = \{\mathsf{x} \text{ is a motion of } \Omega \,|\, \det(\nabla_p\mathsf{x}) = 1,\ \mathscr{S}_\epsilon(\phi(\cdot,t)) = \mathscr{S}_\epsilon(\phi_0) \text{ for all } t\in[0,T]\}.$$

Suppose that a motion $\mathsf{x}\in\mathfrak{X}$ is a critical point of the action $\mathscr{A}$. Then

$$\left.\frac{d}{ds}\mathscr{A}(\mathsf{x}^s)\right|_{s=0} = 0$$

for every smooth, one-parameter family of motions x^s with $\mathsf{x}^0 = \mathsf{x}$ and $\mathsf{x}^s(\cdot,T) = \mathsf{x}(\cdot,T)$. Note that $\phi^0 = \phi$ and $v(\cdot,0) = v^*(\cdot,0) = v(\cdot,T) = v^*(\cdot,T) = 0$. By (2.13) and the change of variables formula, we have then

$$\begin{aligned}
0 = \left.\frac{d}{ds}\mathscr{A}(\mathsf{x}^s)\right|_{s=0} &= \int_0^T\int_\Omega \mathsf{x}_t\cdot\left.\frac{d}{ds}\mathsf{x}^s_t\right|_{s=0}dp + \left.\frac{d}{ds}\mathscr{G}_\epsilon(\phi^s)\right|_{s=0}dt\\
&= \int_0^T\int_\Omega \mathsf{x}_t\cdot v_t\,dp - \int_\Omega \mathscr{G}'_\epsilon(\phi)v^*\cdot\nabla\phi\,dx\,dt\\
&= -\int_0^T\int_\Omega \mathsf{x}_{tt}\cdot v\,dp - \int_\Omega \mathscr{G}'_\epsilon(\phi)v^*\cdot\nabla\phi\,dx\,dt\\
&= -\int_0^T\int_\Omega (u_t + u\cdot\nabla u - \mathscr{G}'_\epsilon(\phi)\nabla\phi)\cdot v^*\,dx.
\end{aligned}$$

Since x^s was arbitrary, we know that $u_t + u\cdot\nabla u - \mathscr{G}'_\epsilon(\phi)\nabla\phi$ lies in the kernel (with respect to the $L^2(\Omega)$ inner product) of the tangent space to $\mathfrak{X}$. Since $\mathscr{S}_\epsilon(\phi^s)$ is constant in s and $\det(\nabla_p\mathsf{x}^s) = 1$, we also know from (2.13) that then there are Lagrange multipliers $\lambda(t)$ and $\mu(t)$ and a function $\tilde{p} : \Omega\times[0,T]\to\mathbb{R}$ for which

$$u_t + u\cdot\nabla u - \mathscr{G}'_\epsilon(\phi)\nabla\phi = \lambda(t)\nabla\tilde{p} + \mu(t)\mathscr{S}'_\epsilon(\phi).$$

Furthermore, the fact that $\det(\nabla_p x(\cdot,t)) = 1$ implies that $\nabla \cdot u = 0$. Defining $p = -\lambda(t)(\tilde{p} + \phi)$ along with (2.11) finally gives the unregularized system

$$u_t + u \cdot \nabla u + \nabla p = (\mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi))\nabla\phi \tag{2.15}$$

$$\nabla \cdot u = 0 \tag{2.16}$$

$$\phi_t + u \cdot \nabla\phi = 0. \tag{2.17}$$

Eqs. (2.15)–(2.17) are in general difficult to solve (individually or as a coupled system) due to the lack of dissipative terms. To remedy this numerical and theoretical difficulty, we arrive at (2.2)–(2.4) by adding $\nu\Delta u$ and $\gamma(\mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi))$ to (2.15) and (2.17) respectively for $\mu, \gamma > 0$. In order to modify the transport equation (2.17) for ϕ, one must carefully choose regularization terms which guarantee that the system satisfy the second law of thermodynamics, as is discussed in the next section.

2.3. Energetic self-consistency

Suppose u, and ϕ are suitably smooth solutions of (2.2)–(2.7). Then the following dissipation law holds:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\int_\Omega |u|^2\,\mathrm{d}x + \mathscr{G}_\epsilon(\phi)\right) = -\nu\int_\Omega |\nabla u|^2\,\mathrm{d}x - \gamma \times \int_\Omega |\mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi)|^2\,\mathrm{d}x. \tag{2.18}$$

An immediate corollary of this inequality is that the kinetic energy of the fluid and the Helfrich energy $\mathscr{G}_\epsilon(\phi)$ remain bounded by the initial data independently of time. Furthermore, the total energy is decreasing in time due to viscous damping and the artificial relaxation. This fact is the premise of the existence theory for this system, see [42] for details.

Let $\xi = \mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi)$. To derive (2.18), we first multiply Eq. (2.2) by u and integrate by parts to find

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\int_\Omega |u|^2\,\mathrm{d}x + \int_\Omega \nu|\nabla u|^2\,\mathrm{d}x = \int_\Omega \xi u \cdot \nabla\phi\,\mathrm{d}x.$$

On the other hand, since $\mathscr{V}(\phi) = \mathscr{V}(\phi_0)$ and $\mathscr{S}_\epsilon(\phi) = \mathscr{S}_\epsilon(\phi_0)$ are constant in t,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{G}_\epsilon(\phi) &= \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{G}_\epsilon(\phi) + \lambda(t)\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{V}(\phi) + \mu(t)\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}_\epsilon(\phi)\\ &= \int_\Omega \xi\phi_t\,\mathrm{d}x = -\int_\Omega \gamma\xi^2 + \xi u\cdot\nabla\phi\,\mathrm{d}x.\end{aligned}$$

Summing the above two equations yields (2.18).

3. Simulation

We have implemented numerical methods for the solution of the coupled system (2.2)–(2.4) with spectral spatial discretizations and semi-implicit time discretizations, using penalty methods rather than Lagrange multipliers. Usual convergence tests have been performed to ascertain the convergence of the numerical solutions. The details are to be reported elsewhere. Here, we merely present results of a single experiment, in which we take a $64 \times 64 \times 64$ grid on a square cube, and $\epsilon = 0.2454$, with a time step $\Delta t = 3 \times 10^{-7}$. The initial membrane is taken to be a relatively flat disc with its volume kept at a value -202.21, and the surface area at 45.99. The fluid velocity is initially given by $u_0 = \left(0, 0, 50\pi\,\mathrm{e}^{-48(x^2+y^2)/\pi^2}\right)$ in x, y, z coordinates. We used periodic boundary condition in the x and y directions and a Dirichlet boundary condition along the z direction which is compatible with the initial velocity field.

In Fig. 3.1, the dynamic shape deformation of the initial membrane is illustrated through snapshots at different time steps (both cutting view and full 3d views of the membrane shapes are shown).

The purpose of this simple numerical experiment is to illustrate the effectiveness of the coupled system and the energetic variation approach. The complex topological changes during the time evolution are well captured in the simulation. This simulation does not take into account the detailed physical transition from the spherical to the toroidal topology as our model phase field Navier–Stokes system is a simplification of the more complex physical situation, but the numerical simulation is faithful to hydrodynamic interaction of the vesicle and fluid through the dissipation and exchange of kinetic energy and Helfrich energy. For this particular simulation, by the generalized Gauss–Bonnet theorem for singular surfaces, one can argue that the energetic contributions from the total Gaussian curvature do not change before, after and during the topological transition. Yet, a model which takes into account the energy of topology of the membrane, as in (1.1), would be desirable for more general topological transformations. Such a model can be constructed, for instance, by modifying (2.1) by the addition of a phase field approximation of the Euler characteristic as described in [16].

4. Formal asymptotics

In this section we combine the self-consistent exchange of energy given by the energy law (2.18) with a formal asymptotic assumption on the solution structure of the phase field ϕ. We will show that the system then converges to a sharp interface formulation given by the force (1.5) and a zero traction boundary condition.

The plan is as follows. First we expand $\mathscr{G}_\epsilon(\phi)$ in powers of ϵ. Then, a uniform energy bound of $\mathscr{G}_\epsilon(\phi)$ in terms of the initial data given by (2.18) implies that the interfacial thickness of the phase field is uniform. Then, if the phase field additionally satisfies the transport equation (2.4) (assuming $\gamma \ll \epsilon^3$), as we will show in this section, the velocity field has zero traction at the surface and that the force due to $\mathscr{G}_\epsilon(\phi)$ (given on the right-hand side of (2.2))

$$\left(\mathscr{G}_\epsilon'(\phi) + \lambda(t) + \mu(t)\mathscr{S}_\epsilon'(\phi)\right)\nabla\phi$$

converges to (1.5).

Let us assume that $\Sigma(t) \subset \mathbb{R}^3$ is a smooth, closed surface evolving smoothly in time, and $d(x,t)$ be the distance to $\Sigma(t)$ defined by

$$d(x,t) = \mathrm{dist}\{x, \Sigma(t)\} = \inf_{z\in\Sigma(t)} |x - z|.$$

For sufficiently small ϵ, suppose that there are functions $\theta : \{(x,t) \in \Sigma(t) : t \in [0,T]\} \to \mathbb{R}_+$, $Q_1, Q_2 : \Omega \times [0,T] \to \mathbb{R}$ and $Q : \mathbb{R} \to \mathbb{R}$ independent of ϵ for which

$$\phi(x,t) = Q\left(\frac{d(x,t)\theta(x,t)}{\epsilon}\right) + \epsilon Q_1(x,t) + \epsilon^2 Q_2(x,t) + \cdots. \tag{4.1}$$

The phase field profile is $Q = Q(x)$, ϵ is the interfacial thickness and Q_1 and Q_2 are higher order terms. The function $\theta(x,t)$ measures the variation in local interfacial thickness for $x \in \Sigma(t)$. A more general two-scale expansion has been considered recently in [36] which generalized the analysis in [35] in the absence of the fluid flow. We elect to work with (4.1) to avoid technical complications. The following calculations are performed in a neighborhood of $\Sigma(t)$ where $d(x,t)$ is smooth. We extend θ in this neighborhood of $\Sigma(t)$ so that

$$|\nabla d| = 1, \quad \nabla d \cdot \nabla\theta = 0. \tag{4.2}$$

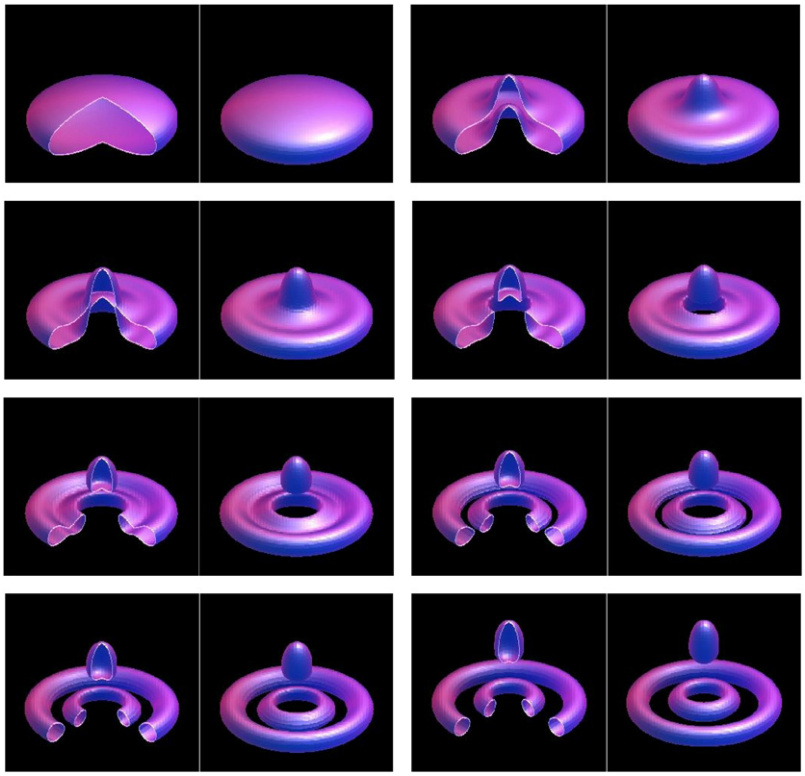

Fig. 3.1. An elliptical disc is flushed by a fluid jet. The snapshots are taken at time $t = 0.0000, 0.0099, 0.0109, 0.0114, 0.0139, 0.0163, 0.0183, 0.0257$ (left to right, then top to bottom).

Formally expanding (2.1) in powers of ϵ,

$$\mathscr{G}_\epsilon(\phi) = \frac{1}{\epsilon^3}\mathscr{G}_{\epsilon,-3}(\phi) + \frac{1}{\epsilon^2}\mathscr{G}_{\epsilon,-2}(\phi) + \cdots$$

we define (where $Q(\cdot) = Q(d(\cdot)\theta(\cdot)/\epsilon)$)

$$\mathscr{G}_{\epsilon,-3}(\phi) = \frac{1}{2c_0}\int_\Omega \left(\ddot{Q}(\theta^2-1)\right)^2 \,\mathrm{d}x \tag{4.3}$$

$$\mathscr{G}_{\epsilon,-2}(\phi) = \frac{1}{2c_0}\int_\Omega \left(\ddot{Q} - Q(Q^2-1)\right)^2 \,\mathrm{d}x \tag{4.4}$$

$$\mathscr{G}_{\epsilon,-1}(\phi) = \frac{1}{c_0}\int_\Omega \dot{Q}^2(\Delta d - 2\kappa(x))^2 \,\mathrm{d}x. \tag{4.5}$$

See Section 1.3 of [35] for details in the expansion.

Proposition 4.1. *Given ϵ sufficiently small, suppose u and ϕ are solutions of (2.2)–(2.7) with ϕ_0 chosen so that $\mathscr{G}_\epsilon(\phi_0)$ be bounded independently of ϵ and ϕ satisfies (4.1). Then*

(1) $\mathscr{G}_{\epsilon,-3}(\phi) = \mathscr{G}_{\epsilon,-2}(\phi) = 0$;
(2) $\theta \equiv 1$ *and* Q *is a solution of* $\ddot{Q} - Q(Q^2-1) = 0$;
(3) $Q_1 \equiv 0$;
(4) $\mathscr{G}_{\epsilon,j} = O(\epsilon)$ *for* $j = 0, 1, \ldots$;
(5) $\lim_{\epsilon\to 0}\mathscr{G}_{\epsilon,-1} = \mathscr{H}_0(\Sigma(t))$.

Proof. We fix a positive number M so that $\|u_0\|^2_{L^2(\Omega)} + G_\epsilon(\phi_0) < M$ for all sufficiently small ϵ. By (2.18), $G_\epsilon(\phi(t)) < M$ for all $t \geq 0$ and in particular,

$$0 \leq \mathscr{G}_{\epsilon,-3}(\phi(t)) \leq (M + O(\epsilon^{-2}))\epsilon^3$$

for all $t > 0$ and all sufficiently small ϵ. This implies the first part of (1). It then follows that

$$0 \leq \mathscr{G}_{\epsilon,-2}(\phi(t)) \leq (M + O(\epsilon^{-1}))\epsilon^2,$$

which implies the second part of (1).

Since the integrands of $\mathscr{G}_{\epsilon,-3}$ and $\mathscr{G}_{\epsilon,-2}$ are positive, we infer that

$$\ddot{Q}^2(\theta^2-1)^2 = \left(\ddot{Q} - Q(Q^2-1)\right)^2 = 0$$

for all $(x, t) \in \Omega \times [0, T]$. Using the boundary conditions on ϕ and the fact that $d(x, t)$ is non-constant in a neighborhood of $\Sigma(t)$, we get (2). Other conclusions, (3), (4) and (5), can be found in Theorems 2.1, 2.2 and 4.1 of [35]. □

Now, from (2.4) we have

$$2\dot{Q}\ddot{Q}(d_t + u\cdot\nabla d) + \epsilon\dot{Q}^2\nabla d\cdot\nabla u\cdot\nabla d = O(\epsilon^2).$$

Sending ϵ to zero, the lowest order term must be zero, but this does not necessarily imply that the distance function is transported by the velocity field since $\dot{Q}$ is zero at the surface. The next term in the expansion must also be zero, so that the velocity field has zero compression normal to the surface. Combining this fact with the incompressibility condition (2.3), we see that velocity also has zero compression tangential to the surface, that is,

$$n(x)\cdot\nabla u(x)\cdot n(x) = \sum_{i=1}^{2}\tau_i(x)\cdot\nabla u(x)\cdot\tau_i(x) = 0 \tag{4.6}$$

for an orthonormal frame $\{n, \tau_1, \tau_2\}$ of the tangent plane of $\Sigma(t)$ at x. Moreover, to show that the limit of (2.2)–(2.4) as ϵ vanishes is a two-phase flow with a zero traction condition on the velocity field and an interfacial force given by (1.5), we compute the limit on the right-hand side of (2.2). First we need the following

Proposition 4.2 (*Integration by Parts*). *Let Σ be a smooth, compact surface without boundary. For a smooth vector field v, smooth scalar fields f and g and smooth surface Σ, one has the following formulae:*

$$\text{(i)}\quad \int_\Sigma \nabla_\Sigma\cdot v\,\mathrm{d}S = -\int_\Sigma 2Hv\cdot n\,\mathrm{d}S, \tag{4.7}$$

$$\text{(ii)}\quad \int_\Sigma \Delta_\Sigma fg\,\mathrm{d}S = \int_\Sigma f\Delta_\Sigma g\,\mathrm{d}S. \tag{4.8}$$

Eq. (4.7) is the first variation formula while (4.8) follows by two applications of the former identity, see [22].

We treat the three terms on the right-hand side of (2.2) separately. Let v be a smooth, compactly supported, divergence free vector field. Following the calculation in Theorem 4.2 of [35], the incompressibility condition (2.3) and Proposition 4.2, we get

$$\begin{aligned}\lim_{\epsilon\to 0}\int_\Omega \mathscr{G}'_\epsilon(\phi)\nabla\phi\cdot v\,\mathrm{d}x &= \int_\Sigma \Delta_\Sigma H v\cdot n - \nabla_\Sigma(H^2-K)\cdot v\\ &= \int_\Sigma \Delta_\Sigma H v\cdot n + 2H(H^2-K)v\cdot n - (H^2-K)\nabla_\Sigma\cdot v\,\mathrm{d}S\\ &= \int_\Sigma (\Delta_\Sigma H + 2H(H^2-K))v\cdot n - (H^2-K)n\cdot\nabla v\cdot n\,\mathrm{d}S\end{aligned}$$

where the last term is zero provided that v is chosen from a test space appropriate for the boundary condition (4.6).

We may also adopt the derivations in [35], to get that the Lagrange multipliers are bounded uniformly with respect to ϵ. We find that, by choosing a subsequence, the remaining body force terms on the right-hand side of (2.2) converge to a linear sum of the mean curvature vector and normal vector.

5. Alternative Eulerian formulations

In this section we contrast the phase field EVA presented in this paper with another Eulerian formulation, the level set method. Strictly speaking, the phase field method also adopts a level set formulation, although we refer to the formulations given in [43] when speaking of the level set method. We will show that in analogy with (2.18), a level set formulation also satisfies the self-consistent exchange of kinetic energy with the average Helfrich energy over all levels, (5.4). Contrary to the phase field approach though, it remains to be investigated how one could regularize the coupled level set system, in particular the transport equation (5.1) for the level set function ρ, so as not to significantly affect the validation of (5.4). An existence theory may thus be more difficult to establish in comparison with that for the phase field approach where the artificial regularization given by the right-hand side of Eq. (2.4) provides additional dissipation in the energy law (2.18) [42].

Let the level set indicator function ρ satisfy the transport equation

$$\rho_t + u\cdot\nabla\rho = 0 \tag{5.1}$$

and be sufficiently smooth. Consider the average of mean curvature energy of all level sets

$$\mathscr{F}(\rho) = \int_{\mathbb{R}}\int_{\Sigma_{t,c}} H^2\,\mathrm{d}S\,\mathrm{d}c \tag{5.2}$$

where $\Sigma_{t,c} = \{x : \rho(x,t) = c\}$ is a smooth two-dimensional hypersurface without boundary for almost every $c\in\mathbb{R}$, it will be shown in what follows that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\rho) &= \int_{\mathbb{R}}\int_{\Sigma_{t,c}} (\Delta_\Sigma H + 2H(H^2-K))u\cdot n\,\mathrm{d}S\,\mathrm{d}c\\ &= \int_\Omega (\Delta_\Sigma H + 2H(H^2-K))u\cdot\nabla\rho\,\mathrm{d}x.\end{aligned} \tag{5.3}$$

Here H, K and ∇_Σ are defined as in Section 1 with $n = \nabla\rho/|\nabla\rho|$. The last equality follows from the co-area formula [44]. Suppose now that u satisfies the momentum equation (2.2) where we replace the body force on the right-hand side by the term $(\Delta_\Sigma H + 2H(H^2-K))\nabla\rho$ defined on Ω. Multiplying this new momentum equation by u and integrating over Ω and adding the resulting expression to (5.3), we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\int_\Omega |u|^2\,\mathrm{d}x + \mathscr{F}(\rho)\right) + \nu\int_\Omega |\nabla u|^2\,\mathrm{d}x = 0. \tag{5.4}$$

We now verify (5.3) below. A similar treatment may be found in [45]. We reiterate these results here with a slightly different class of test functions and an albeit shorter calculation. First we need the following

Proposition 5.1. *Let $\rho\in C_0^4(\Omega)$ and f and g be smooth functions on Ω. Then*

$$\int_\Omega |\nabla\rho|\Delta_\Sigma fg\,\mathrm{d}x = \int_\Omega |\nabla\rho| f\Delta_\Sigma g\,\mathrm{d}x.$$

Proof. By Sard's theorem, almost every level of ρ is a smooth, two-dimensional hypersurface without boundary. By the co-area formula and Proposition 4.2,

$$\begin{aligned}\int_\Omega |\nabla\rho|\Delta_\Sigma fg\,\mathrm{d}x &= \int_{\mathscr{R}}\int_{\{\rho=c\}} \Delta_\Sigma fg\,\mathrm{d}S\,\mathrm{d}c\\ &= \int_{\mathscr{R}}\int_{\{\rho=c\}} f\Delta_\Sigma g\,\mathrm{d}S\,\mathrm{d}c = \int_\Omega |\nabla\rho| f\Delta_\Sigma g\,\mathrm{d}x.\end{aligned}$$

□

From the definitions for n and H given in Section 1,

$$\begin{aligned}2H_t &= -\frac{\mathrm{d}}{\mathrm{d}t}\nabla\cdot n = -\frac{\mathrm{d}}{\mathrm{d}t}\nabla\cdot(\nabla\rho|\nabla\rho|^{-1})\\ &= -\nabla\cdot(\nabla\rho_t|\nabla\rho|^{-1} - \nabla\rho\nabla\rho_t\cdot\nabla\rho|\nabla\rho|^{-3}).\end{aligned}$$

From (5.1), setting $\rho_t = -u\cdot\nabla\rho = -u\cdot n|\nabla\rho|$ and using the definition of ∇_Σ from Section 1 to show that $|\nabla\rho|\nabla_\Sigma|\nabla\rho|^{-1} = n\cdot\nabla n$ gives

$$\begin{aligned}2H_t &= \nabla\cdot(\nabla(u\cdot\nabla\rho)|\nabla\rho|^{-1} - \nabla\rho\nabla\rho\cdot\nabla(u\cdot\nabla\rho)|\nabla\rho|^{-3})\\ &= \nabla\cdot(\nabla(u\cdot n) - nn\cdot\nabla(u\cdot n) - (u\cdot\nabla\rho)\nabla_\Sigma|\nabla\rho|^{-1})\\ &= \Delta_\Sigma(u\cdot n) - n\cdot\nabla n\cdot\nabla(u\cdot n) + \nabla\cdot((u\cdot n)n\cdot\nabla n)\\ &= \Delta_\Sigma(u\cdot n) + (u\cdot n)\nabla\cdot(n\cdot\nabla n)\\ &= \Delta_\Sigma(u\cdot n) + (u\cdot n)\mathrm{tr}(\nabla n)^2 + (u\cdot n)n\cdot\nabla(\nabla\cdot n)\end{aligned}$$

where we have collected terms into $\Delta_\Sigma(u\cdot n)$ and made the appropriate cancellations after multiple applications of the product rule. Finally, noting (1.4) and using $\nabla\cdot n = -2H$ once more, we get the desired identity

$$2H_t = \Delta_\Sigma(u\cdot n) + (u\cdot n)(4H^2-2K) - 2(u\cdot n)n\cdot\nabla H. \tag{5.5}$$

To verify (5.3), first we apply the co-area formula and (5.1) to get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\rho) &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}}\int_{\Sigma_{c,t}} H^2\,\mathrm{d}S\,\mathrm{d}c = \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega |\nabla\rho|H^2\,\mathrm{d}x\\ &= \int_\Omega -|\nabla\rho|^{-1}\nabla\rho\cdot\nabla(\rho_t) + 2|\nabla\rho|HH_t\,\mathrm{d}x\\ &= \int_\Omega -n\cdot\nabla(u\cdot\nabla\rho)H^2 + 2|\nabla\rho|HH_t\,\mathrm{d}x.\end{aligned}$$

Using (5.5) in the second term, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\rho) = \int_\Omega \big[&-H^2 n\cdot\nabla(u\cdot\nabla\rho) + |\nabla\rho|H(\Delta_\Sigma(u\cdot n)\\ &+(u\cdot n)(4H^2-2K) - 2(u\cdot n)n\cdot\nabla H)\big]\,\mathrm{d}x.\end{aligned}$$

Integrating by parts in the first term (while noting that $u = 0$ on $\partial\Omega$) and using $\nabla\cdot n = -2H$, we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\rho) = \int_\Omega \big[&|\nabla\rho|(n\cdot\nabla(H^2) - 2H^3)(u\cdot n)\\ &+|\nabla\rho|H(\Delta_\Sigma(u\cdot n) + (u\cdot n)(4H^2-2K)\\ &-2(u\cdot n)n\cdot\nabla H)\big]\,\mathrm{d}x.\end{aligned}$$

Now the last term cancels with the first because $2H\nabla H = \nabla(H^2)$; collecting terms and using (5.4) to integrate Δ_Σ by parts, we finally have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\rho) = \int_\Omega |\nabla\rho|(u\cdot n)(\Delta_\Sigma H + 2H(H^2-K))\,\mathrm{d}x = \int_{\mathcal{R}}\int_{\Sigma_{t,c}} (u\cdot n)(\Delta_\Sigma H + 2H(H^2-K))\,\mathrm{d}S\,\mathrm{d}c.$$

The above variation, commonly known as variation with respect to the domain, is in fact the usual Lagrangian evaluated over the special test class $\{v\cdot\nabla\rho : v\in C_0^\infty(\Omega:\mathbb{R}^n)\}$.

6. Conclusion

In this paper, a coupled system of equations is presented as a model for the deformation of three-dimensional vesicle membranes in the fluid fields. The vesicle configuration is determined by the competition between the elastic bending energy, with prescribed bulk volume and surface area, and the surrounding fluid velocity fields. The configuration in turn affects the fluid fields. Our derivation is mostly based on an energetic variational approach, with a diffuse interface method. The method transforms the membrane deformation from a Lagrangian description to an Eulerian description and leads to an induced constitutive equation that ensures the energy dissipation. In a very general ansatz, we have shown that, as the regularization parameter goes to zero, the asymptotic limit of the coupled system is consistent with a sharp interface dynamics. Preliminary numerical simulations also support the effectiveness of using our coupled system to study the interaction of the vesicle membrane with the background incompressible fluid. For brevity, only the case of a constant density is considered for the fluid, and only a simplified version of the Helfrich energy is analyzed, without incorporating contributions such as those from the spontaneous curvature and Gaussian curvature. Extensions to more general cases can be made and they will be investigated in subsequent works. More extensive numerical tests and studies of other effects, such as the interaction with electro-magnetic fields, will be also investigated in the future.

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