Semipermeable, Multicomponent Vesicles in Stokes Flow

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Abstract

We apply a high-order boundary integral equation method to simulate multicomponent, semipermeable membranes in various Stokes flows. Our multicomponent vesicles are representative of cell membranes containing aquaporins and are only permeable to water. This semipermeability is important for many biophysical processes including cell migration and cell rupture. Our semipermeability model depends on the membrane forces where the fluid flux is proportional to the pressure drop. The multicomponent model uses the Cahn-Hilliard equation to allow for phase separation between different lipid species. We consider vesicles in quiescent flow and shear flow.

Introduction

Vesicles are deformable capsules that are:

- Submerged in and filled with an incompressible viscous fluid
- Resist bending
- Locally inextensible
- Used to model biomembranes such as red blood cells

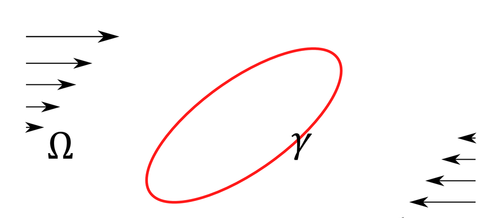


Figure 1: *Ω is the unbounded fluid domain and γ is the vesicle membrane. In addition to the vesicle-induced flow, a shear flow is imposed in the far field.*

Governing Equations

Following the work of Sohn et al, JCP, 2010, we define the lipid energy as

$$E^T = \frac{a}{\epsilon}\int_\gamma \left(f(u) + \frac{\epsilon^2}{2}|\nabla_\Sigma u|^2\right) ds, \quad \text{free energy,}$$
$$f(u) = \frac{1}{4}u^2(1-u)^2, \quad \text{double well potential,}$$

and the membrane energy as

$$E^B = \int_\gamma \left(\frac{1}{2}b(u)\kappa^2 + \sigma\right) ds, \quad \text{bending energy,}$$
$$b(u) = b_{\max}u + b_{\min}(1-u), \quad \text{bending modulus.}$$

The fluid and vesicle equations are

$$\begin{aligned}
\mu\Delta\mathbf{u} &= \nabla p, & \mathbf{x}\in\Omega, &\quad \text{conservation of momentum,}\\
\nabla\cdot\mathbf{u} &= 0, & \mathbf{x}\in\Omega, &\quad \text{conservation of mass,}\\
[[\mathbf{u}]] &= 0, & \mathbf{x}\in\Omega, &\quad \text{velocity continuity,}\\
[[T]]\mathbf{n} &= \mathbf{f}, & \mathbf{x}\in\gamma, &\quad \text{force balance,}\\
\frac{d\mathbf{x}}{dt} &= V\mathbf{n} + T\mathbf{s} + \boxed{\beta(\mathbf{f}\cdot\mathbf{n})\mathbf{n}} & \mathbf{x}\in\gamma, &\quad \text{dynamic equation for the vesicle,}\\
V &= \mathbf{u}\cdot\mathbf{n}, \quad T = \mathbf{u}\cdot\mathbf{s} & &\quad \text{normal and tangential velocities}\\
\mathbf{f} &= (b(u)\kappa\mathbf{n})_{ss} - \frac{3}{2}(b(u)\kappa^2\mathbf{s})_s + & \mathbf{x}\in\gamma, &\quad \text{membrane force,}\\
&\quad \left(\frac{a}{\epsilon}\left(f(u) - \frac{\epsilon^2}{2}u_s^2\right)\mathbf{s}\right)_s - (\sigma\mathbf{s})_s,
\end{aligned}$$

and have the conditions

$$\begin{aligned}
\nabla_\gamma\cdot\frac{d\mathbf{x}}{dt} &= 0, & \mathbf{x}\in\gamma, &\quad \text{local inextensibility,}\\
\mathbf{u}(\mathbf{x}) &= \dot\gamma(x_2, 0), & |\mathbf{x}|\to\infty, &\quad \text{far-field condition.}
\end{aligned}$$

We do a change of variables to the θ-L formulation. After this change of variables, the dynamics of θ and L are governed by

$$\frac{\partial\theta}{\partial t} = -\left(V + \boxed{\beta(\mathbf{f}\cdot\mathbf{n})}\right)_s + \kappa T,$$
$$\frac{dL}{dt} = \left(T_s + \kappa\left(V + \boxed{\beta(\mathbf{f}\cdot\mathbf{n})}\right)\right)L,$$

with the inextensibilty condition

$$T_s + \kappa\left(V + \boxed{\beta(\mathbf{f}\cdot\mathbf{n})}\right) = 0.$$

To reduce the stiffness of the system, we extract the dominant terms in the governing equations at small spatial scales.

$$V \sim \frac{b_{\max}}{4\bar{s}_\alpha^2}\mathcal{L}[\theta_{\alpha\alpha\alpha}] + \boxed{\beta\left(\frac{b_{\max}}{4\bar{s}_\alpha^3}\theta_{\alpha\alpha\alpha}\right)},$$

where

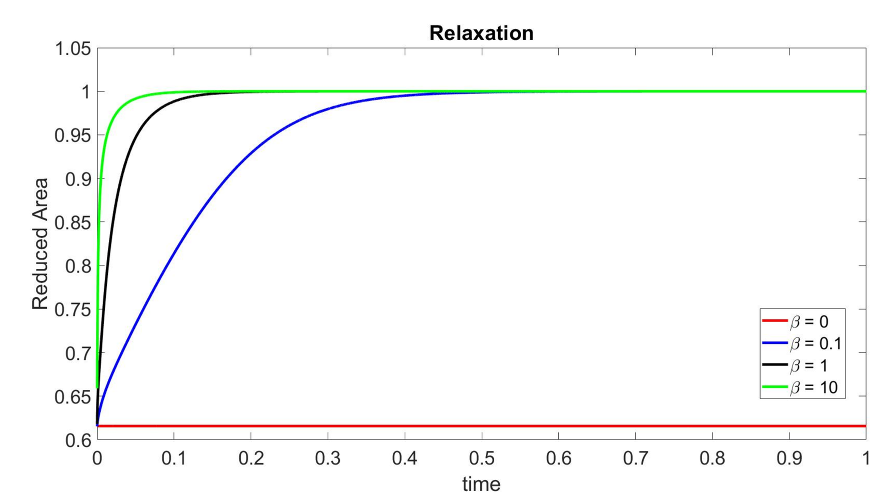
$$\mathcal{L}[\mathbf{f}](\alpha) = \frac{1}{\pi}\int_0^{2\pi}\log\left(2\left|\sin\left(\frac{\alpha-\alpha'}{2}\right)\right|\right)\mathbf{f}(\alpha')\,d\alpha'.$$

The reduced area of the vesicle is defined as A/A_0 where A is the area of the vesicle and A_0 is the area of a circle with the same length as γ.

Numerical Examples

Semipermeable, Single-Component Vesicle in a Quiescent Flow

The steady-state shape is always a circle.



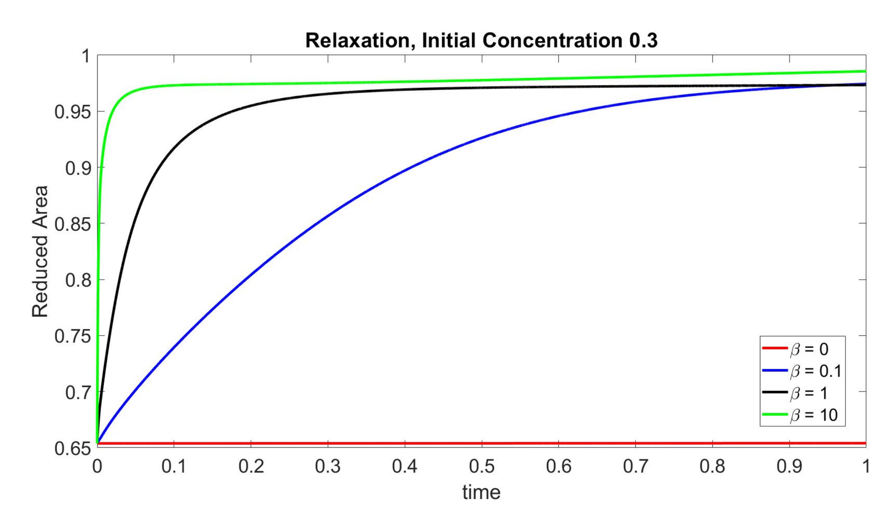
$$J = \frac{b}{2}\int_\gamma \kappa^2\,ds + \sigma\left(\int_\gamma ds - L\right)$$
$$\frac{\delta J}{\delta\gamma} = 0 \quad\Rightarrow\quad \kappa(s) = \frac{2\pi}{L},\ \sigma = \frac{2\pi^2}{L^2}$$

The vesicle area satisfies

$$\frac{dA}{dt} = \beta\int_\gamma\left(\frac{\kappa^3}{2} - \kappa\sigma\right)ds.$$

Semipermeable, Multicomponent Vesicle in a Quiescent Flow

The steady-state shape is no longer a circle.



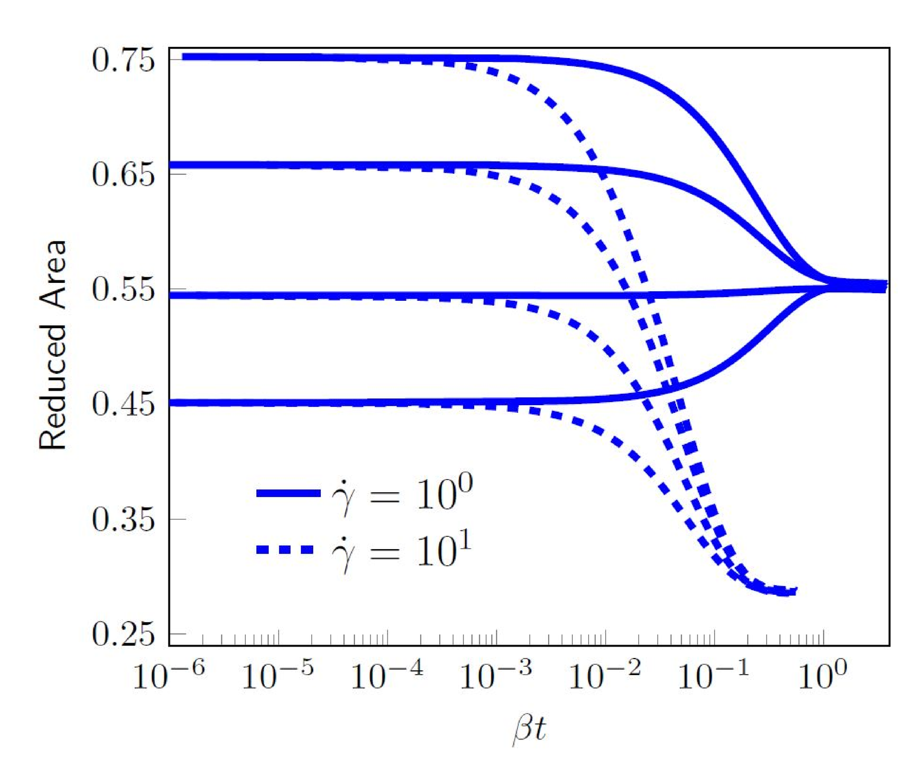
Initial concentration

$$u(\alpha,0) = \bar{u} + \lambda(3\cos(\alpha) + 0.5\cos(3\alpha) + 0.5\cos(4\alpha))$$
$$\bar{u} = 0.3, \quad \lambda = 0.05, \quad \alpha\in[0,2\pi]$$

with bending modulus

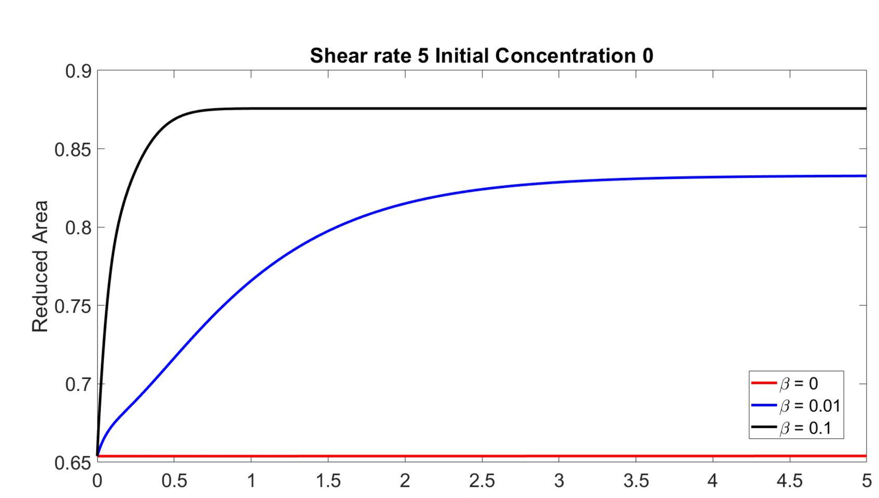
$$b(u) = (1-u)b_{\min} + ub_{\max}$$

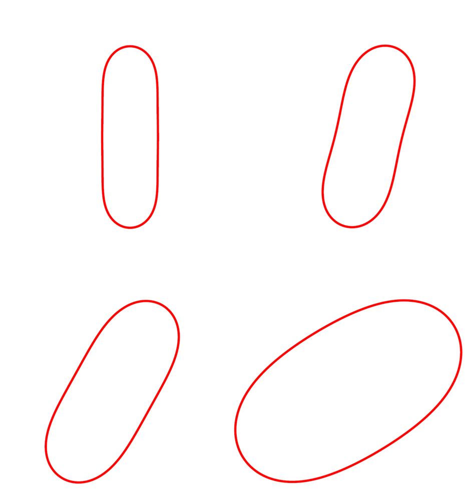
Semipermeable, Single-Component Vesicle in Shear Flow



- The reduced area of a semipermeable vesicle in a shear flow initialized with four different reduced areas.
- The final reduced area is independent of the initial reduced area, but depends on the shear rate.
- Higher shear rates result in lower final reduced areas.

Semipermeable, Single-Component Vesicle in Shear Flow





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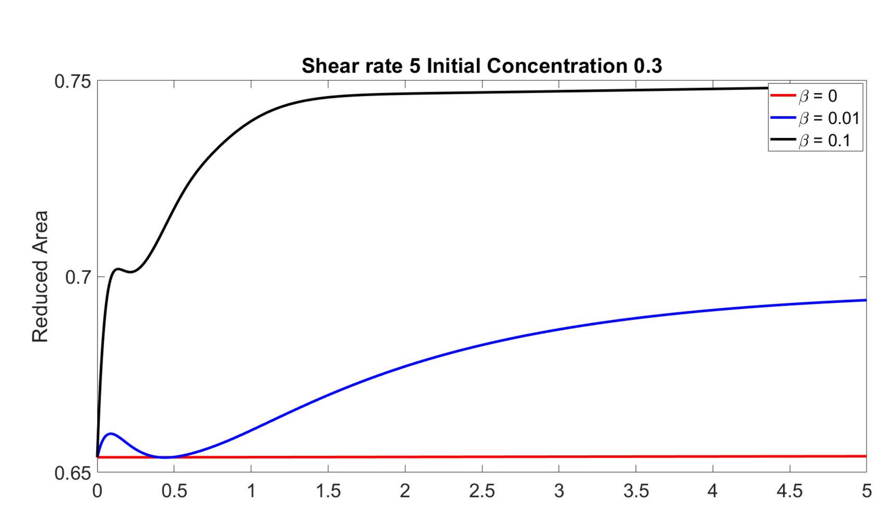

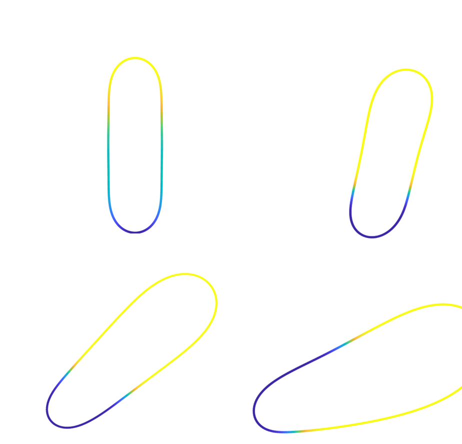

Discussion

- Have developed integral equation methods to simulate multicomponent semipermeable vesicles.
- In a quiescent flow, single-component vesicles inflate to a circle, but multicomponent vesicles inflate to non-circular shapes.
- In a shear flow, semipermeable vesicles tank tread or tumble depending on the lipid concentration.