Hydrodynamics of a Multicomponent Vesicle Under Strong Confinement

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Abstract

The biophysical lipid bilayer membrane (such as a vesicle) often consists of multiple species of macromolecules such as cholesterol, surface proteins, surfactants, and different lipids. I use the phase-field model for a multicomponent lipid membrane and implement the hydrodynamics with a boundary integral code. The simulations covered in this poster show that the multicomponent structure results in fundamentally different behaviors than a single component vesicle.

Introduction

What is a Vesicle?

Vesicles are deformable (2D) capsules that:

- are submerged in and filled with an incompressible viscous fluid
- are governed by hydrodynamic interactions with walls, resistance to bending (with lipid-dependent modulus), and the inextensibility condition.
- have multi-component phase seperated membranes.
- are proxies for many biophysical cells, such as red blood cells.
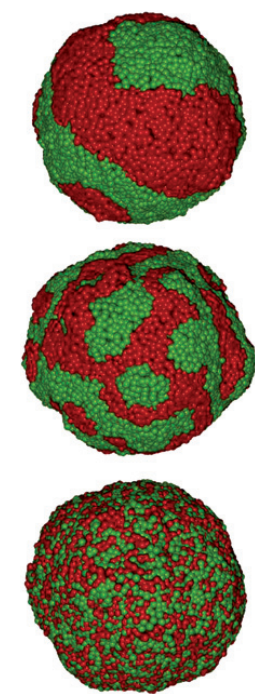
Bagatolli and Kumar, Soft Matter, 2009
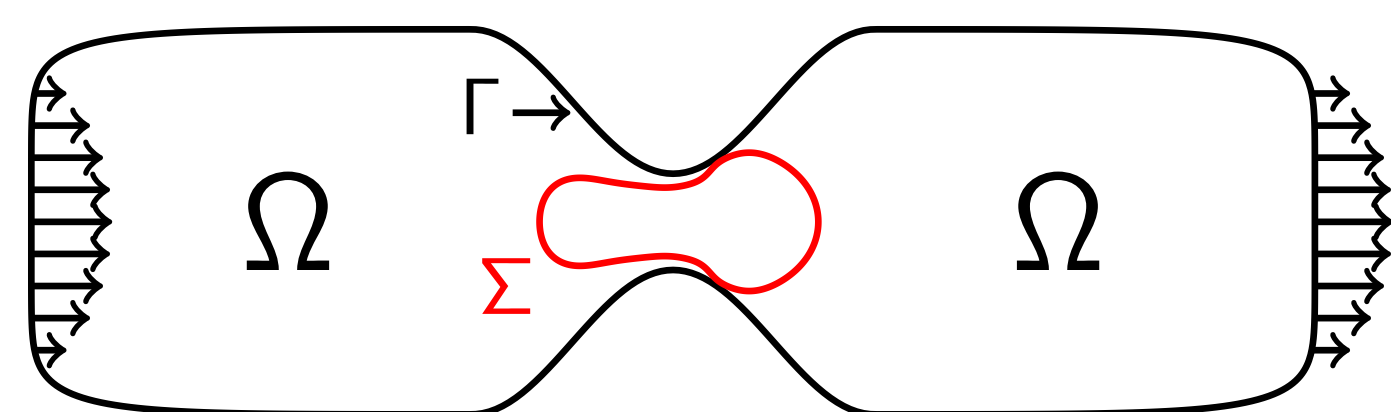
Hydrodynamic Model

Fluid Equations

$\mu \Delta \mathbf{u} = \nabla p,$	Cons. momentum,
$\nabla \cdot \mathbf{u} = 0,$	Cons. mass,
$[\![\mathbf{u}]\!] = \mathbf{0},$	Continuity,
$[\![\mathbf{T}]\!]\mathbf{n} = \mathbf{f}_B + \mathbf{f}_T + \mathbf{f}_P,$	Force balance,
$\mathbf{T} = -p\mathbf{I} + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right),$	Stress tensor.

Vesicle Boundary Conditions

$\dfrac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x})$	No-slip
$\mathrm{div}_\Sigma \mathbf{u} = 0$	Inextensibility

Wall Boundary Conditions

$$\mathbf{u}(\mathbf{x}) = \mathbf{U}(\mathbf{x}), \quad \mathbf{x} \in \Gamma$$

Figure 1: Ω is the fluid domain with boundary Γ and Σ is the vesicle membrane. In addition to the vesicle-induced flow, a Poiseuille flow is imposed at the intake and outtake.

Multicomponent Vesicle Forces

Phase Energy

$$E_P = \frac{a}{\epsilon} \int_\Sigma \left(f(u) + \frac{\epsilon^2}{2}|\nabla_\Sigma u|^2 \right) ds$$

$$f(u) = \frac{1}{4}u^2(1-u)^2$$

Bending and Tension Energies

$$E_B = \int_\Sigma \frac{1}{2}b(u)\kappa^2 \, ds$$

$$E_T = \int_\Sigma \sigma \, ds$$

Original Bending Stiffness [3]

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

New Bending Stiffness

$$b(u) = b_{\min} + \frac{b_{\max}}{2}\left(1 - \tanh\left(3u - \frac{1}{2}\right)\right)$$

Membrane Forces

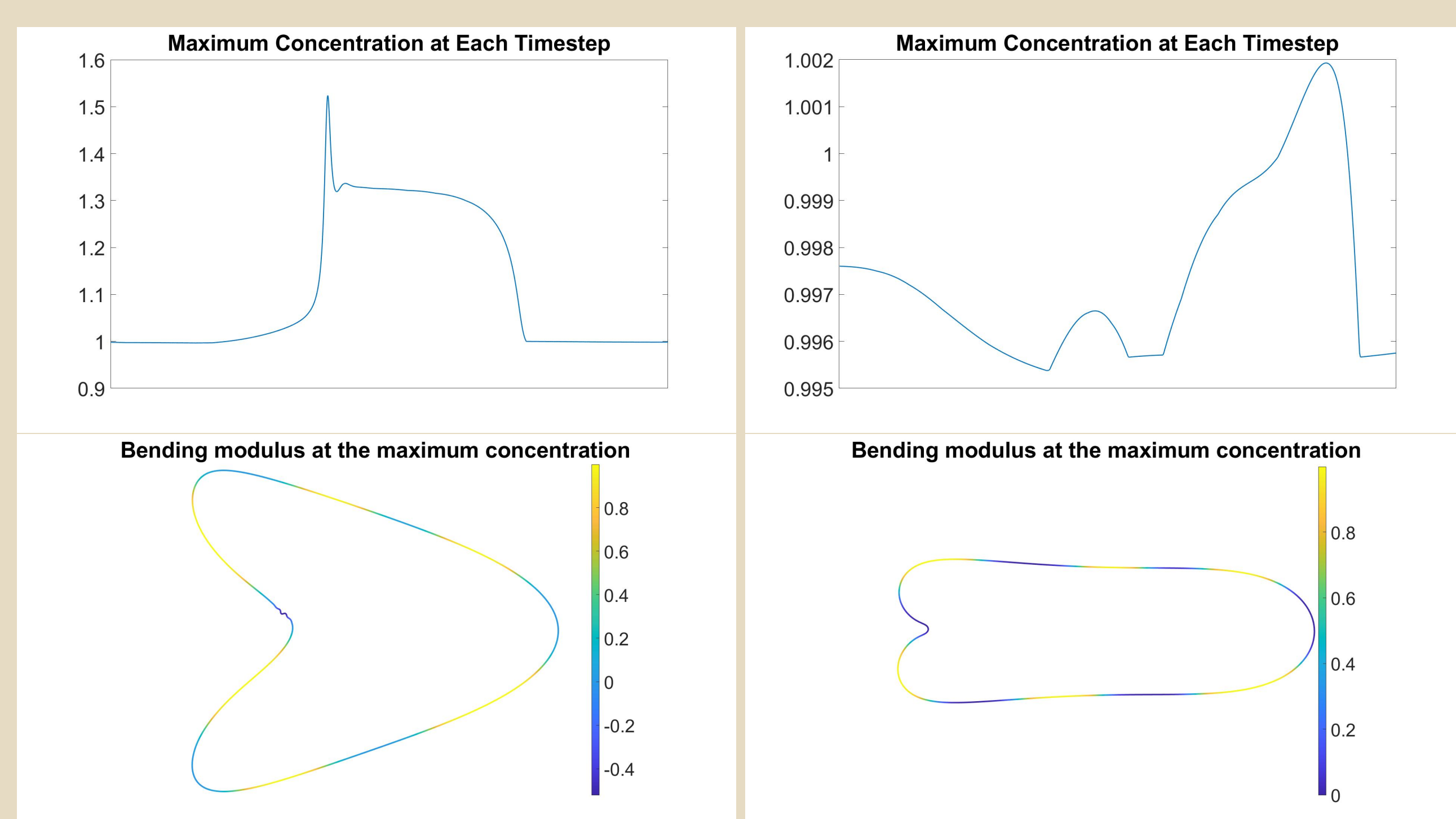|	
$\mathbf{f}_P = \left(\dfrac{a}{\epsilon}\left(f(u) - \dfrac{\epsilon^2}{2}u_s^2\right)\mathbf{s}\right)_s,$	phase,
$\mathbf{f}_T = (\sigma \mathbf{s})_s,$	tension,
$\mathbf{f}_B = -(b(u)\kappa \mathbf{n})_{ss} - \dfrac{3}{2}(b(u)\kappa^2 \mathbf{s})_s,$	bending.

Model Features

- Lipid species phase separate
- Total lipid mass is conserved
- Bending modulus remains bounded between $b_{\min}$ and $b_{\max}$

Numerical Examples

### The Importance of the New Bending Model

Figure 2: Under strong confinement, the lipid species concentration exceeds 1 or falls below 0 since the double well potential does not have hard boundaries. This is problematic for the linear bending modulus since it leads to an unphysical negative bending stiffness. Even though the shape stabilizes, this leads to a drastic increase in the error.

The Membrane Energies
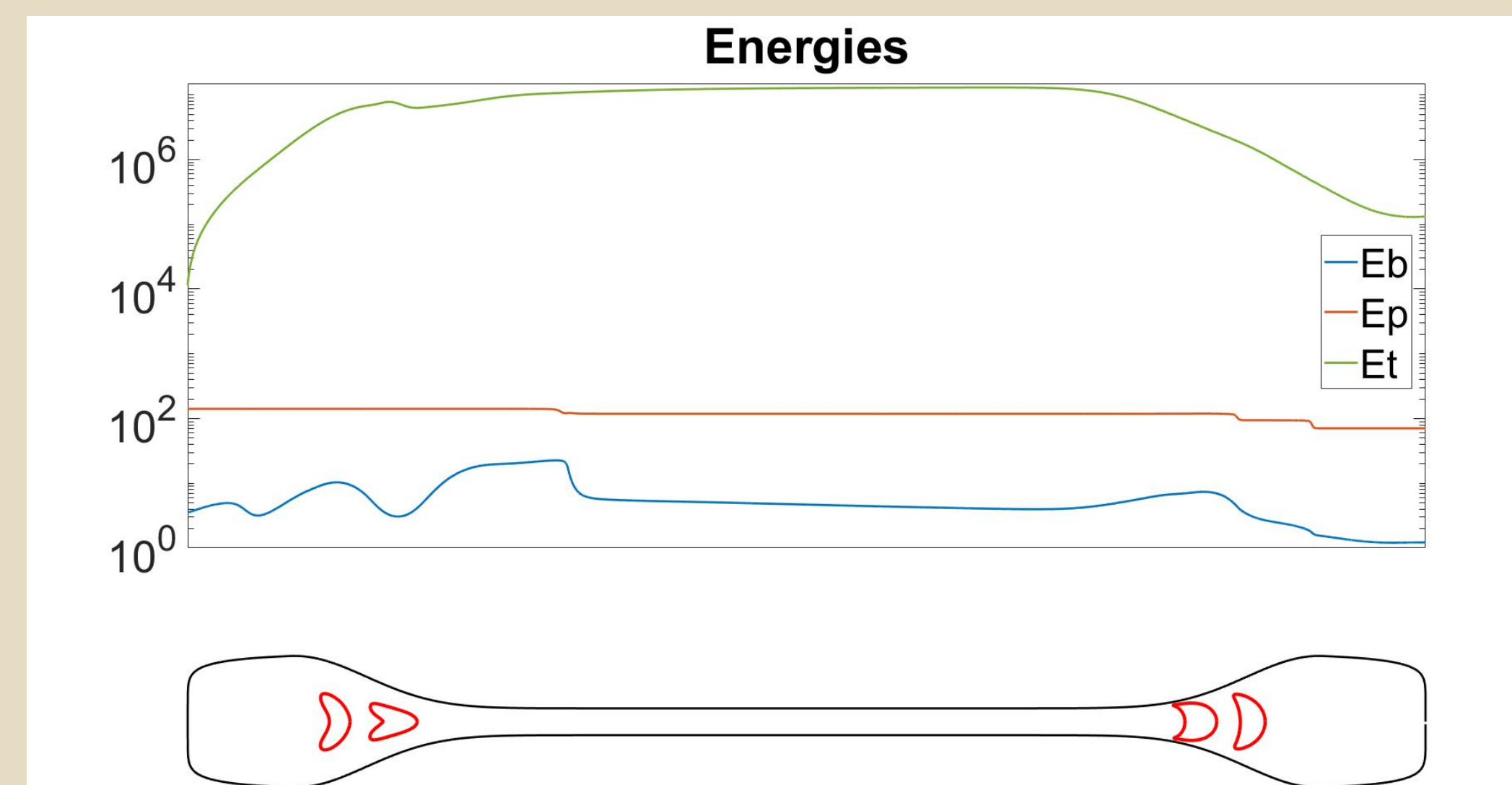
Figure 3: Membrane bending (blue), tension (green), and phase (red) energies. As the vesicle enters the channel, the tension increases by 3 orders of magnitude and dominates the membrane energy until the vesicle exits the channel. Once the vesicle exits the channel, the tension decreases along with the phase energy (phase separation), and the bending energy decreases as the vesicle relaxes.

Shape of Mulicomponent Vesicles
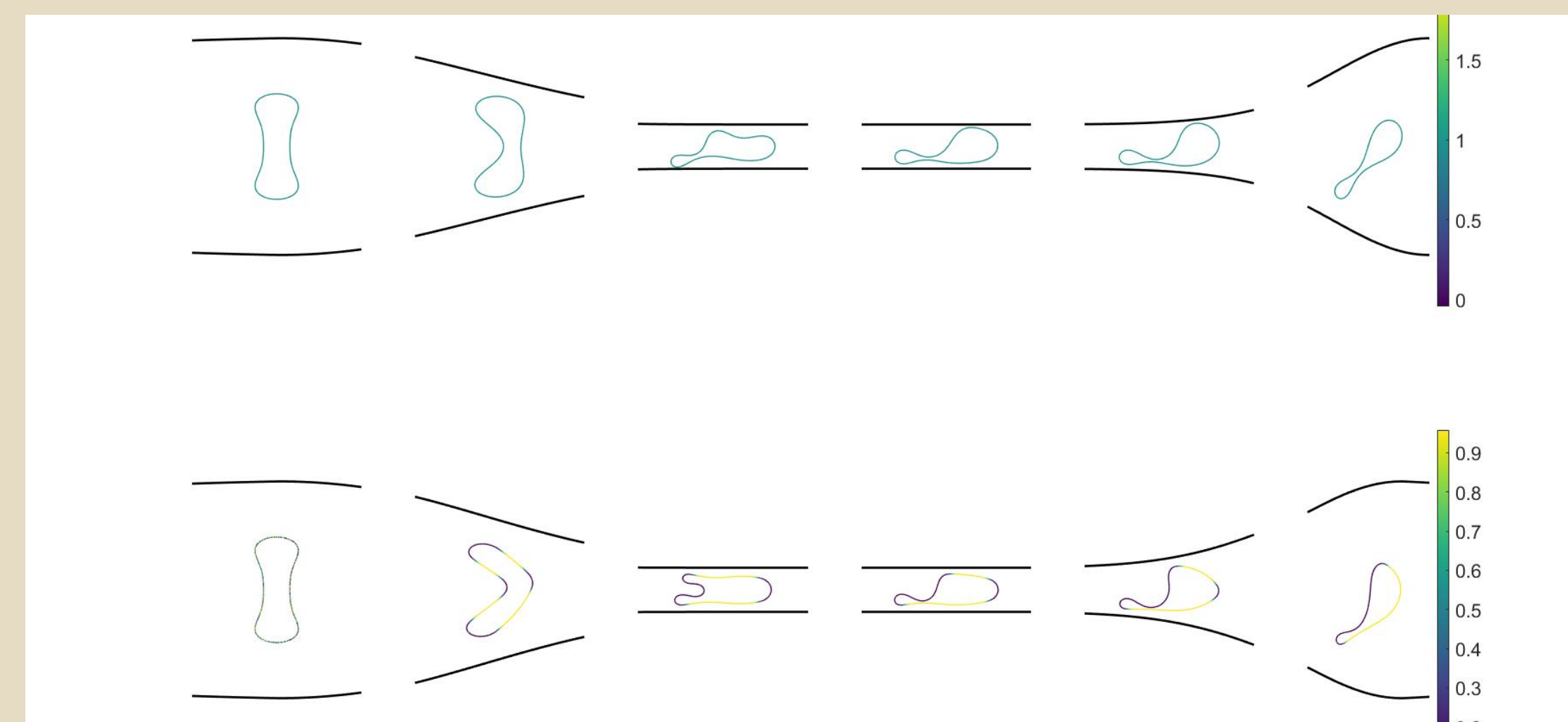
Figure 4: At low flow rates ($U_{\max} = 0.5\mu m/s$) the multicomponent vesicles and single-component vesicles have vastly different shapes.

Migration Speed of Multicomponent Vesicles
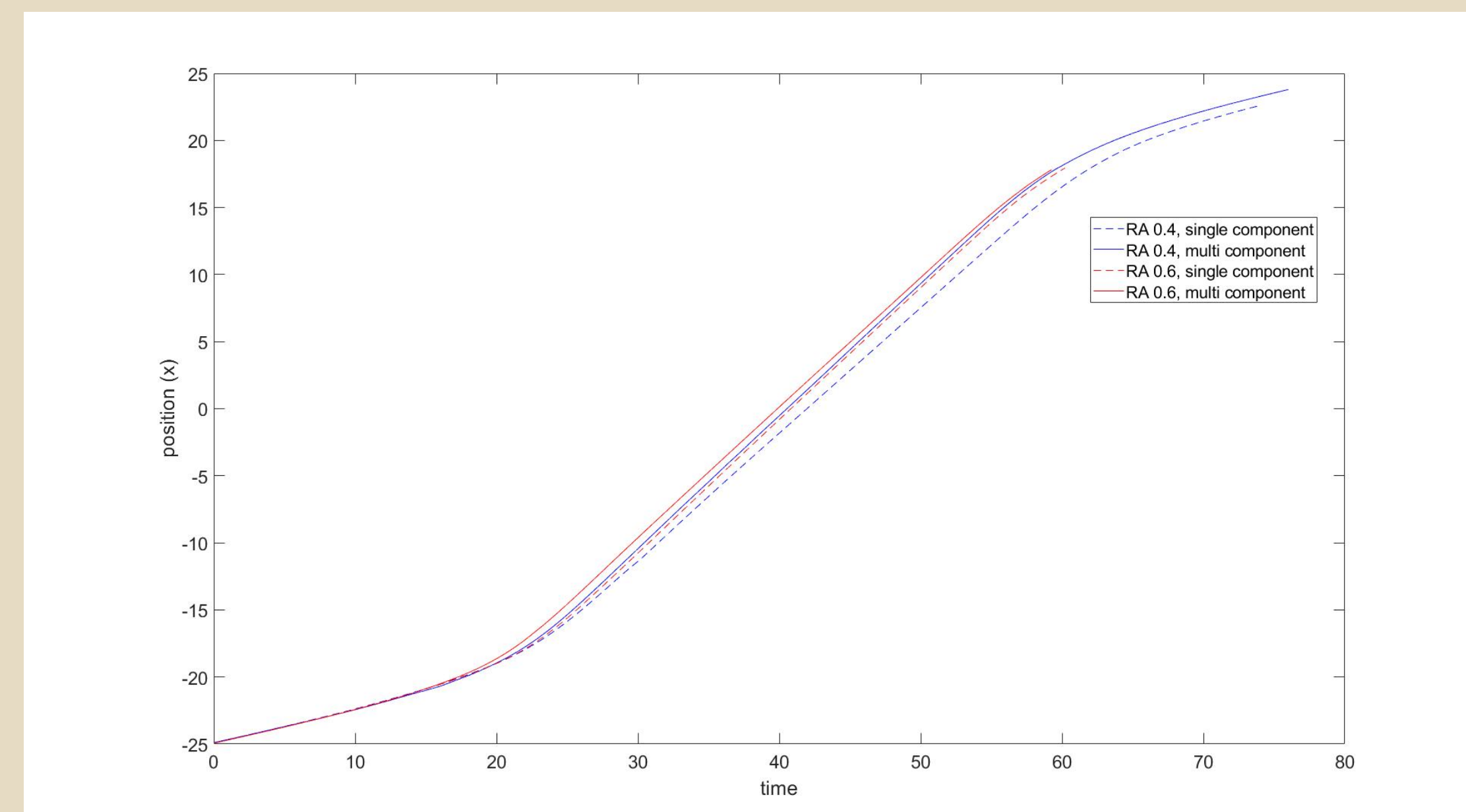
Figure 5: Location vs. time for two different reduced areas and single- vs. multicomponent. The multi-component vesicles move through the channel quicker than their single-component counter parts.

Conclusions

- Vesicles in strong confinement experience strong deformations that result in phenomena, such as permeability [2], that many models ignore.
- A new bending model guarantees the bending modulus is bounded between $b_{\min}$ and $b_{\max}$.
- In a closely-fitting channel, lipid species phase separation occurs slower than in the wider regions since the membrane tension dominating the dynamics.
- For small flow rates, a multicomponent vesicle's shape is different than a single-component vesicle's shape.
- Multicomponent vesicles move through the closely fitting channel quicker than the single-component vesicles.
- Future direction includes investigating long time transient behavior such as tank treading and phase treading [1].

References

[1] Kai Liu, Gary R. Marple, Shuwang Li, Shravan Veerapaneni, and John Lowengrub. Dynamics of a multicomponent vesicle in shear flow. *Soft Matter*, 13:3521–3531, 2017.

[2] Bryan Quaife, Ashley Gannon, and Y.-N. Young. Hydrodynamics of a Semipermeable Vesicle Under Flow and Confinement. *Physical Review Fluids*, 6:073601, 2021.

[3] Jin Sun Sohn, Yu-Hua Tseng, Shuwang Li, Axel Voigt, and John S. Lowengrub. Dynamics of multicomponent vesicles in a viscous fluid. *Journal of Computational Physics*, 229:119–144, January 2010.