Semi-Permeable Deformable Vesicles in a Viscous Fluid

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Abstract

Aquaporins are channels located on cell membranes that facilitate the movement of water into and out of a cell at much higher rates than osmosis. Studies have demonstrated that this transport across cell membranes plays a critical role in cell movement. We apply a high-order boundary integral equation method to simulate the motion of a single vesicle with a semi-permeable deformable membrane in a variety of Stokes flows. The dynamics are compared with impermeable vesicles.

Introduction

Vesicles are deformable capsules that are:

- Submerged in and filled with an incompressible viscous fluid
- Resist bending
- Locally inextensible
- Used to model red blood cell suspensions

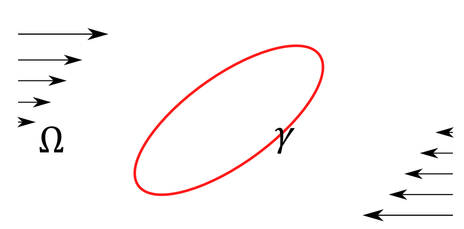

Figure 1: *Ω is the unbounded fluid domain and γ is the vesicle membrane. In addition to the vesicle-induced flow, a shear flow is imposed in the far field.*

Governing Equations

The fluid and vesicle equations are

$$
\begin{aligned}
-\nabla p + \mu \Delta \mathbf{u} &= 0, && \mathbf{x} \in \Omega && \text{conservation of momentum,}\\
\nabla \cdot \mathbf{u} &= 0, && \mathbf{x} \in \Omega && \text{conservation of mass,}\\
[[T]]\mathbf{n} &= \mathbf{f}, && \mathbf{x} \in \gamma && \text{force balance,}\\
\mathbf{f} &= \mathbf{f}_B + \mathbf{f}_T, && \mathbf{x} \in \gamma && \text{membrane force,}\\
\mathbf{f}_B &= -\kappa_b \mathbf{x}_{ssss}, && \mathbf{x} \in \gamma && \text{bending force,}\\
\mathbf{f}_T &= (\sigma \mathbf{x}_s)_s, && \mathbf{x} \in \gamma && \text{tension force,}\\
\mathbf{u} - \frac{d\mathbf{x}}{dt} &= \beta(\mathbf{f}\cdot\mathbf{n})\mathbf{n}, && \mathbf{x} \in \gamma && \textbf{slip boundary condition,}\\
\nabla_\gamma \cdot \frac{d\mathbf{x}}{dt} &= 0, && \mathbf{x} \in \gamma && \text{local inextensibility.}
\end{aligned}
$$

A boundary integral equation formulation places all unknowns on the vesicle interface

$$
\begin{aligned}
\frac{d\mathbf{x}}{dt} &= -\beta(\mathbf{f}\cdot\mathbf{n})\mathbf{n} + \mathcal{S}[\mathbf{f}](\mathbf{x}), && \mathbf{x} \in \gamma\\
\mathcal{S}[\mathbf{f}](\mathbf{x}) &= \frac{1}{4\pi\mu}\int_\gamma \left(-\log\rho + \frac{\mathbf{r}\otimes\mathbf{r}}{\rho^2}\right)\mathbf{f}(\mathbf{y})\,ds_{\mathbf{y}}, && \mathbf{r} = \mathbf{x}-\mathbf{y}, \quad \rho = ||\mathbf{r}||.
\end{aligned}
$$

The area is not constant and satisfies

$$\frac{dA}{dt} = \beta \int_\gamma (\mathbf{f}\cdot\mathbf{n})\,ds. \qquad (\star)$$

Numerical Methods

- Discretize the vesicles at collocation points
- Fourier differentiation to compute $\mathbf{f}_B$ and $\mathbf{f}_T$
- Evaluate the weakly-singular single layer potential $\mathcal{S}[\mathbf{f}](\mathbf{x})$ with Alpert quadrature
- Time adaptive spectral deferred correction that applies IMEX-Euler twice per time step

Numerical Examples

Quiescent Flow

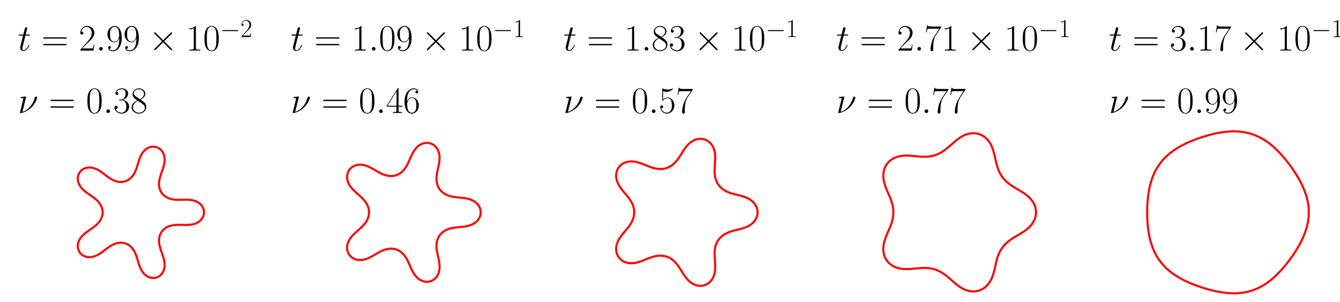

Figure 2: *The evolution of a semi-permeable vesicle in a quiescent flow to a circle.*

Shear Flow

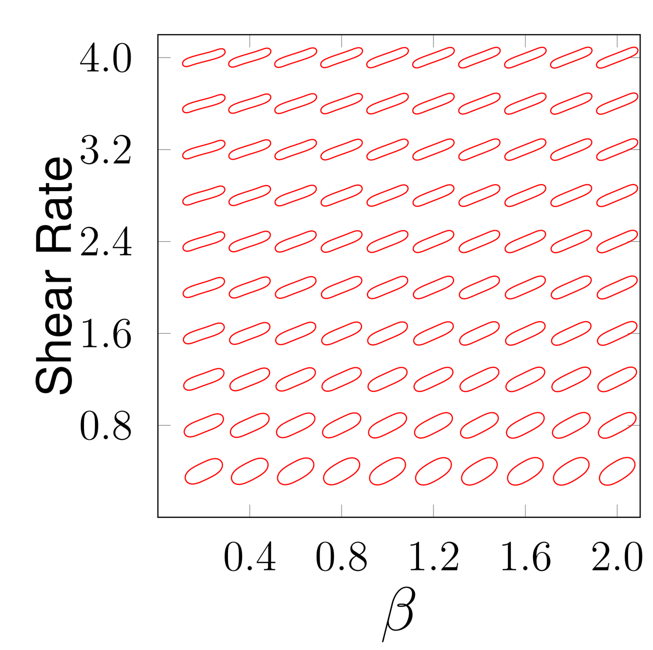

Figure 3: *The steady-state shape of a semi-permeable vesicle in a shear flow. After reaching a steady area, the vesicles undergo tank treading dynamics. The most slender tank treading shapes observed occurred at small β and large shear rates.*

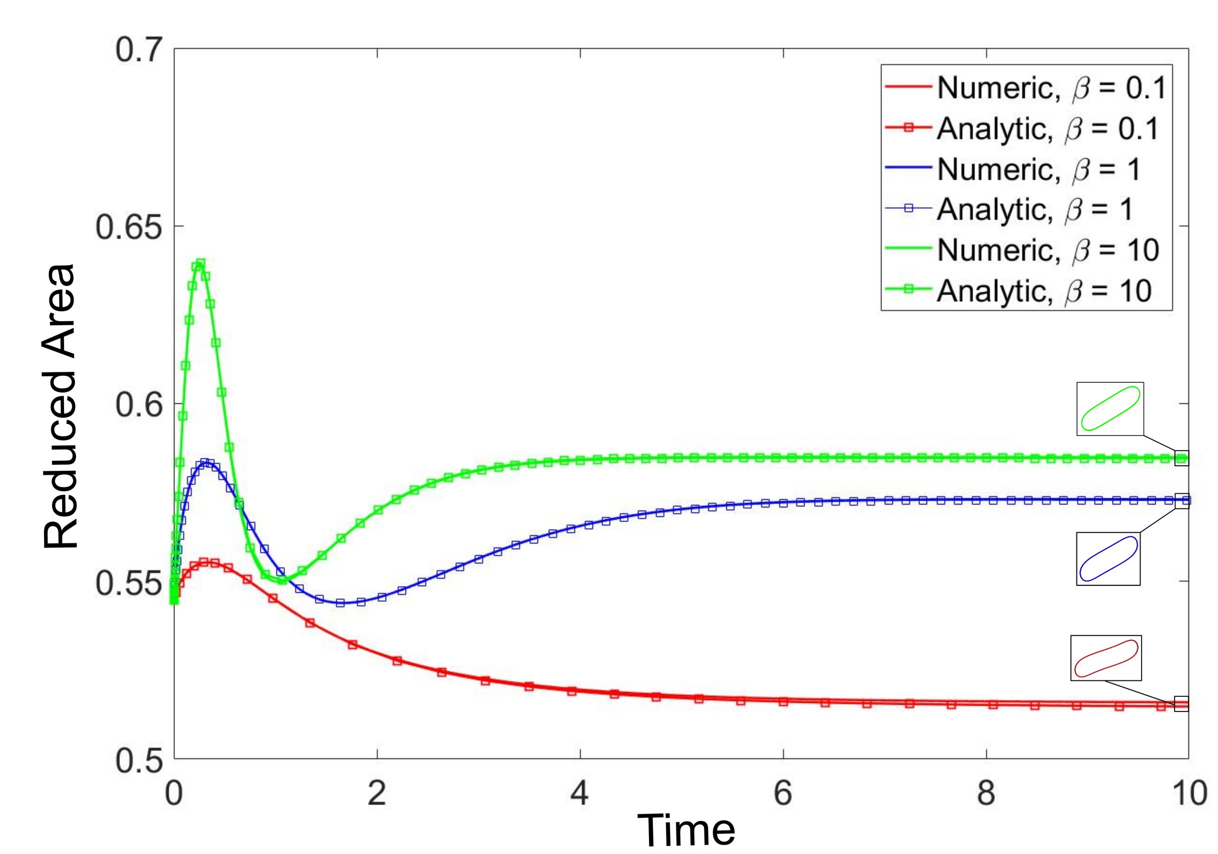

Figure 4: *There is an asymptotic reduced area (RA) that depends on the water flux coefficient, β. The analytic expression ($\star$) is used to predict the RA values of each curve with first order accuracy.*

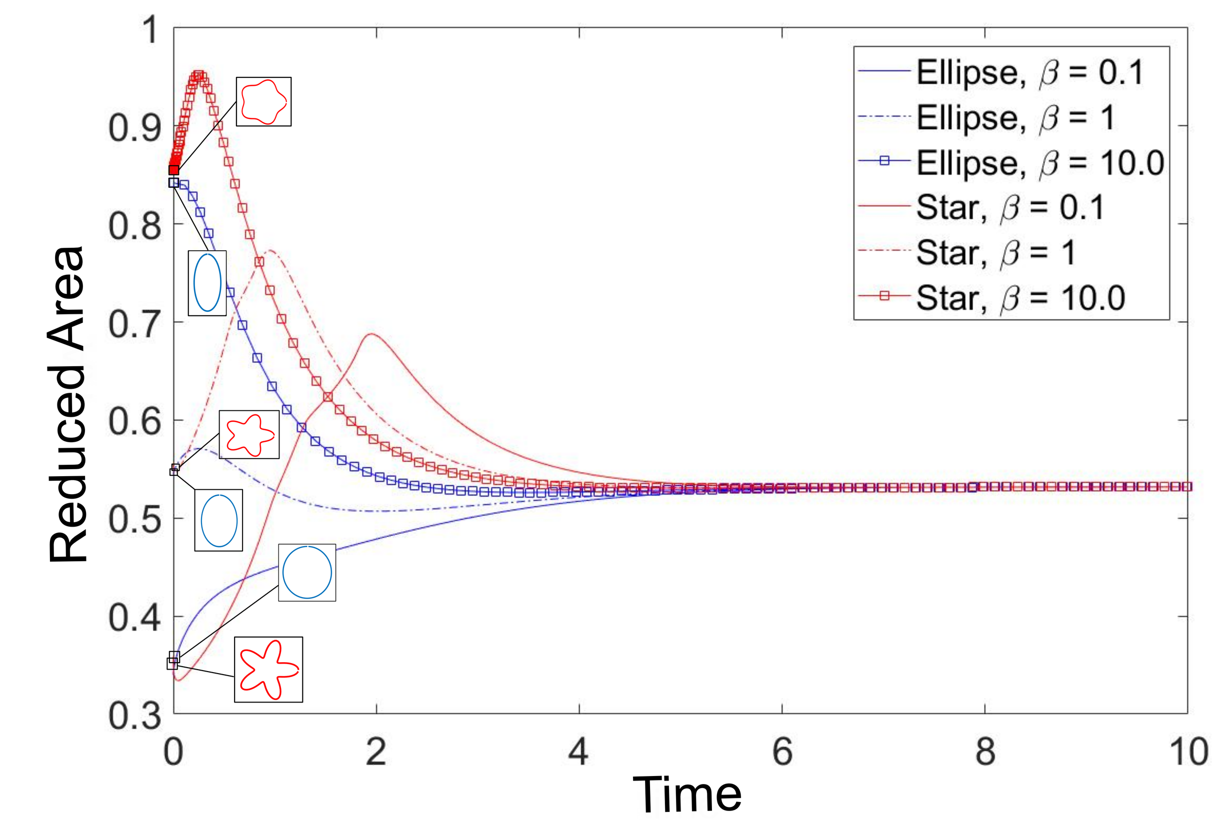

Figure 5: *The final RA does not depend on the initial RA or vesicle shape. In this figure, $\beta = 1$ and all vesicles have the same length.*

β	RA_0	RA_T	IA_T
0.1	0.55	0.51	0.30
1	0.55	0.57	0.40
10	0.55	0.58	0.46
β	RA_0	RA_T	IA_T
0	0.51	-	0.28
0	0.57	-	0.31
0	0.58	-	0.31

Table 1: *We compare impermeable vesicles with initial RA values equal to the final RA values of a semipermeable vesicle. Semi-permeable vesicles reach higher inclination angles, which can affect the effective viscosity.*

Discussion

- The steady-state shape of a semi-permeable vesicle in a quiescent flow is circular.
- A semi-permeable vesicle in shear flow tank treads.
- The area of the vesicle is characterized by the flux ($\star$).
- The final RA of a semi-permeable vesicle depends on the water flux coefficient and the initial length of the vesicle.
- The final RA of a semi-permeable vesicle does not depend on the initial RA or shape.
- In a shear flow, semi-permeable vesicles tank tread at a different inclination angle than clean vesicles.
- Future work will include a concentration gradient of a solute.

References

[1] Bryan Quaife and George Biros. Adaptive Time Stepping for Vesicle Simulations. *Journal of Computational Physics*, 306:478-499, 2016.

[2] Lingxing Yao and Yoichiro Mori. A numerical method for osmotic water flow and solute diffusion with deformable membrane boundaries in two spatial dimension. *Journal of Computational Physics*, 350:728-746, 2017.