Vesicle dynamics in shear and capillary flows

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INTRODUCTION
The deformation of a vesicle in flow is an important subject not only of fundamental research but also in medical applications. In microcirculation, the deformation of red blood cells reduces the flow resistance of microvessels. The deformability of red blood cells is reduced in some diseases.

We studied the vesicle dynamics using a 3D multi-particle collision dynamics simulation with a dynamically-triangulated membrane model.

SIMULATION METHOD

Multi-Particle Collision Dynamics (MPC) is a particle-based hydrodynamics method, which is also called Stochastic rotation dynamics [1]. The solvent is described as N\(s\) point-like particles of mass \(m\). The MPC algorithm consists of two steps. In the streaming step, the particles move ballistically,

\[ \mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t, \]

where \(\Delta t\) is the time interval between collisions. In the collision step, the particles are sorted into cubic cells and the relative velocities of each particle is rotated in a cell:

\[ \mathbf{v}_i(t+\Delta t) = \mathbf{v}_i(t) + \mathbf{v}_{cm}(t) + \mathbf{v}_{cell}(t), \]

where \(\mathbf{v}_{cm}\) is the velocity of the center of mass of all particles in the cell. The matrix \(\Omega\) rotates velocities by a fixed angle \(\phi\) around an axis chosen randomly. To induce a simple shear flow \((\mathbf{v}_x, \mathbf{v}_y, \mathbf{v}_z)\), we employed Les-Edwards boundary conditions. A gravitation force and no-slip boundary conditions were employed for flow in the cylindrical capillary with radius \(R_{\text{cap}}\).

Membrane modeled by dynamically-triangulated surface [2]. The shape and fluctuations of the membrane are controlled by its curvature elasticity.

\[ \tau = \frac{\kappa R^2}{2} \]

The solvent particles do not penetrate the membrane. We also simulated the vesicle with shear elasticity as a model red blood cell in capillary. We mainly present vesicles with the reduced volume \(V_{\text{red}} = 0.59\), and not coaxial with capillary.

Parameters:
- \(\eta_S\), the viscosity of solvent
- \(\kappa\), bending rigidity
- \(\gamma = \gamma_0 R_{\text{cap}}^3/\kappa\), the reduced shear rate
- \(\eta_{\text{mb}} = \eta_{\text{mb}}^{\text{rel}} R_{\text{cap}}^3/\kappa\), the relative membrane viscosity
- \(\tau = \eta_S R_{\text{cap}}^2/\kappa\), the time unit for capillary flow

CONCLUSION

Simple shear flow [3,4,6]
Vesicles transit from steady tank-treading to unsteady tumbling motion with an increase in membrane viscosity. Shear induces discocyte-to-prolate or prolate-to-discocyte transformation at low or high membrane viscosity, respectively.

Capillary flow [5]
As flow velocity increases, shear-elastic vesicles transit from a non-axisymmetric discocyte to an axisymmetric parachute shape, while fluid vesicles transit from a discocyte to a prolate ellipsoid. Both shape transitions reduce the flow resistance. The critical velocities of the shape transitions are linearly dependent on the bending rigidity and on the shear modulus of the membrane.

\[ \text{Shear rate} = \frac{\text{Transition velocity}}{\text{Capillary flow velocity}} = \frac{\eta_{\text{mb}}}{\eta_S R_{\text{cap}}^3/\kappa} \]

\[ \text{Shape transition} \quad \text{Discocyte} \rightarrow \text{Prolate} \rightarrow \text{Parachute} \]

\[ \text{Transition velocity} \quad \frac{\text{Discocyte}}{\text{Prolate}} \rightarrow \text{Parachute} \]

\[ \text{Parachute} \rightarrow \text{Discocyte} \]

\[ \text{Shape transition} \quad \text{Discocyte} \rightarrow \text{Prolate} \rightarrow \text{Parachute} \]

\[ \text{Parachute} \rightarrow \text{Discocyte} \]

\[ \text{Membrane viscosity} \quad \eta_{\text{mb}} \]

\[ \text{Relative membrane viscosity} \quad \eta_{\text{mb}}^{\text{rel}} \]

\[ \text{Shear modulus} \quad \mu R_{\text{cap}}^2/\kappa T = 112 \]

\[ \text{Shear modulus} \quad \mu R_{\text{cap}}^2/\kappa T = 10 \]

\[ \text{Linear dependence of transition velocities} \quad \mathbf{v}_c \]

(a) fluid and shear-elastic vesicles at \(\mu R_{\text{cap}}^2/\kappa T = 112\),

(b) shear-elastic vesicles at \(\mu R_{\text{cap}}^2/\kappa T = 10\).