MANIPULATING SMALL DROPLETS IN MICROCHANNELS WITH COMPLEX FLUIDS

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I use Blue Waters to engineer complex fluids and soft materials at the nanoscale.
Manipulating particles in microchannels

- filtration
- fractionation
- cell sorting
- oil recovery
- water treatment

How can we systematically engineer these processes?

Di Carlo et al., PNAS 104, 18892 (2007).
Complex fluids
Cross-stream migration

Addition of a viscoelastic component induces migration in Poiseuille flow

What happens when the particles become “small”? 

D'Avino et al., Lab Chip 12, 1638 (2012).
Cross-stream migration at the nanoscale

Brownian motion

Comparable length scales
PEO $R_e \sim 300$ nm


Average force on particles $\langle F_x \rangle$ gives average direction of movement

$\langle F_x \rangle = 0$

$\langle F_x \rangle > 0$

$\langle F_x \rangle < 0$
Mesoscale modeling

- Time scale: fs, ns, μs, ms, s
- Length scale: nm, μm, mm
- Resolution
- Speed

- Atomistic models
- Coarse-grained & mesoscale models
- Constitutive models
Coarse-grained models

- Bond stretch
- Dispersion forces, excluded volume, electrostatics
- Angle bend
- Dihedral twist
What happens if the particles are droplets or cells that deform?

Droplet migration

\[ \mathbf{F} = \mathbf{F}_C + \mathbf{F}_R + \mathbf{F}_D \]

- **Repulsive force**
- **Random force**
- **Drag force**
Why Blue Waters

Large parametric design space

- 4 polymers
- x 3 polymer concentrations
- x 5 flow rates
- x 5 replicas

= Large coarse-grained model

- 384,000 particles
- = 4 GPUs for 48 hours
- (HOOMD-blue)

Blue Waters is the only system available to us with the GPU resources needed!
Droplet in a neat solvent is different from a rigid particle

Droplet shape depends on the local flow

\[ D = \frac{L - B}{L + B} \]

Flow and droplet position depend on polymer concentration

Solution is non-Newtonian for higher polymer concentrations.

Droplet moves inward with increasing polymer concentration.

Conclusions

Polymer solutions can be used to manipulate droplets in microchannels.

Droplet position and shape depend on the polymer solution and flow.

Important for applications like membrane filtration or cell sorting.


All software has been released open source on GitHub: mphoward/azplugins