Computational Study of Fluid Particles:

Dynamics of Drops
Rheology of Emulsions
Mechanics of Biological Cells

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Overview of dissertation

- Navier-Stokes
- Deforming interface
- Front-tracking

Dynamics of drop
- Oscillating extensional flow (OE) *Phys. Fluids*
- Vortex flow *J. Fluid Mech.*

Rheology of emulsion
- Shear flow *Phys. Rev. Letters*

Mechanics of cell
- In unbounded shear *J. Comp. Phys.*
- In shear near a wall
- Cell adhesion...
Emulsions: applications and challenges

- Material
- Energy
- Biology

- Food processing
- Polymer manufacturing
- Oil recovery & refinement
- Blood diagnosis

Interfacial restoring force

Effective stress

Complex microstructure
Dynamic & inertial environment

Iza & Bousmina (2000) J. Rheology

Rheology

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Oscillating extensional (OE) flow

Computer-controlled four-roll mill
Taylor (1932), Bentley & Leal (1986)

- Inertia & time-dependency: less investigated
- Turbulent flow → oscillatory forcing

Stokes flow analysis
Asymptotic: small deformation
Taylor (1932), Cox (1969)
BEM: arbitrary deformation
Rallison & Acrivos (1978)

Drop in oscillating extensional flow

- Amplitude
- Frequency
- Oscillating four-roll mill
Drop deformation and phase in OE flow

Drop in OE: complex 3D flow with moving interface

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

Taylor (1932)

Deformation
Deformation

Computational result

Reduced-order analysis

\[ |X| = \sqrt{\frac{1 + \hat{S}t^2 \hat{Re}^2}{(\hat{k} - \hat{S}t^2 \hat{Re})^2 + \hat{S}t^2}} \]

Re increase

Natural frequency

Frequency

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Resonance breakup

- Efficient energy transfer at appropriate frequency
- Frequency selective breakup in turbulence !!!
- Gas bubble breakup in turbulence
  Risso & Fabre (1998)
**Rheology computation**

Assume dilute emulsion:

Excess stress: \( \sigma_{\text{excess}} = \Phi \sigma_{\text{excess}}^d = -\Phi \Gamma q^d \)

\[ q_d = \frac{1}{V} \int_A \left( nn - \frac{I}{3} \right) dA \]

- **Elastic stress**
  - \( \sim \) flow strain

- **Viscous stress**
  - \( \sim \) flow strain rate

**Interface tensor**

**Drop-shape \( \rightarrow \) Stress**
Rhoelogy in OE flow (Re=0.1)

Modulus (stress/strain)

Phase (behind strain rate)
Negative elasticity ($Re=1$)

Modulus (stress/strain)

- Effective property
- Due to inertia induced microstructure change
- Elastic response in the same direction as forcing

Resonance

$E'$

$E''$

Flow frequency

Negative Elasticity!
Rheology in shear

In Stoke’s flow of emulsions

\[ N_1^{\text{int}} = \sigma_{11} - \sigma_{22} > 0 \]

\[ N_2^{\text{int}} = \sigma_{22} - \sigma_{33} < 0 \]

Choi and Schowalter (1975)
Sign change of normal stress difference

\[ N_{1}^{\text{int}} = \sigma_{11} - \sigma_{22} \]

\[ N_{2}^{\text{int}} = \sigma_{22} - \sigma_{33} \]

Re=0.1 \rightarrow \text{Re}=1.0

\[ Ca = \frac{\mu R_{0} \dot{\gamma}}{\sigma} \]
Cell modeling: membrane and bond

- Lipid-bilayer + network of proteins
- Elastic membrane

Leukocyte (WBC) adhesion

- Molecular bond
- Elastic spring
- Stochastic formation and rupture

http://bme.virginia.edu/ley/
Equilibrium rupture rate $k_r$:

$$k_r = k_{r0} \exp(\gamma F/k_b T)$$  Bell (1987)

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**Sensitivity of rupture rate to forces $\gamma$**

**Deformable particle in shear flow near a wall**

**Hydrodynamic LIFT**

**Pushing particle from wall**

**Leal (1980)**

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**Deformation of particle**

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Summary

• Drop deformation → Rheology

• Oscillating extensional flow (OE) → dynamic & inertial: turbulent flow

• Drop in OE at finite inertia → resonance → breakup in turbulence → negative phase → negative elasticity in emulsion

• Drop in shear at finite inertia → orientation angle > 45° → sign change of normal stress difference in emulsion

• Effects of cell deformation → Lift force → Adhesion
Current activities: High Re two-phase flow

Propulsion /power generation  Fire suppression  Lubrication

Models at various levels of fidelity

High fidelity direct Simulation  Mesoscale CFD Simulation  Dynamic Reduced Order Modeling
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