ALE-FEM for Two-Phase Flows with Surfactants

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Transport processes at fluidic interfaces

DFG SPP 1506

Main Interest

Interfacial flows with/without surfactants

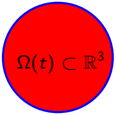
- flows with liquid-liquid (interface) or liquid-gas (free surface) boundaries
- flows with surface active agents (surfactants)
- aim is to develop an accurate and robust numerical scheme for interfacial flows with insoluble/soluble surfactants

Properties

- surfactant (surface active agent) is a substance that lowers the surface/interfacial tension on liquid-gas/liquid-liquid interface
- nonuniform distribution of surfactants on surface/interface induce Marangoni convection

Navier-Stokes Equation

Free surface flow



$$
\begin{aligned}
\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) - \nabla \cdot \mathbb{S}\, (\mathbf{u}, p) &= \rho\, \mathbf{g} && \text{in } \Omega\,(t) \\
\nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega\,(t) \\
\mathbf{u} \cdot \nu &= \mathbf{w} \cdot \nu && \text{on } \Gamma(t) \\
\mathbb{S}(\mathbf{u}, p) \quad \cdot \nu &= \nabla_\Gamma \cdot (\sigma \mathbb{P}_\Gamma) && \text{on } \Gamma(t)
\end{aligned}
$$

$+$initial and appropriate boundary conditions

$$\mathbb{S}\,(\mathbf{u}, p) = \mu\, \mathbb{D}(\mathbf{u}) - p\mathbb{I}, \quad \mathbf{g} = \text{external force field (gravity)}, \quad \sigma = \sigma(c_\Gamma)$$

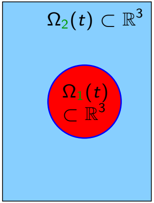
Surfactant dependent surface tension:

$$
\begin{aligned}
\sigma(c_\Gamma) &= \sigma_0 + RT_a(c_{\Gamma,0} - c_\Gamma) && \text{(Henry)} \\
\sigma(c_\Gamma) &= \sigma_0 + c_{\Gamma,0} RT_a \ln(1 - \tfrac{c_\Gamma}{c_{\Gamma,0}}) && \text{(Langmuir)}
\end{aligned}
$$

$\mathbf{u}$ - velocity, p - pressure, t - time, ρ - density, $\mathbf{w}$ - surface velocity, c_Γ - surface surfactant concentration, Γ - free surface/interface, ν - outer normal to Ω , g - gravity, σ - surface tension, $\mathbb{P}_\Gamma$ - projection to tangential plane, μ - dynamic viscosity, σ_0 - reference surface tension, $c_{\Gamma,0}$ - reference concentration, R - ideal gas constant, T_a - absolute temperature

Navier-Stokes Equation

Two-phase flow ($j = 1, 2$)



$$
\begin{aligned}
\rho_j \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) - \nabla \cdot \mathbb{S}_j(\mathbf{u}, p) &= \rho_j \mathbf{g} && \text{in } \Omega_j(t) \\
\nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega_j(t) \\
[|\mathbf{u}|] = 0, \quad \mathbf{u} \cdot \nu &= \mathbf{w} \cdot \nu && \text{on } \Gamma(t) \\
[|\mathbb{S}(\mathbf{u}, p)|] \cdot \nu &= \nabla_\Gamma \cdot (\sigma \mathbb{P}_\Gamma) && \text{on } \Gamma(t)
\end{aligned}
$$

+initial and appropriate boundary conditions

$\mathbb{S}_j(\mathbf{u}, p) = \mu_j \mathbb{D}(\mathbf{u}) - p\mathbb{I}$, $\quad$ $\mathbf{g}$ = external force field (gravity), $\quad$ $\sigma = \sigma(c_\Gamma)$

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$\mathbf{u}$ - velocity, p - pressure, t - time, ρ_j - density, $\mathbf{w}$ - surface velocity, c_Γ - surface surfactant concentration, Γ - free surface/interface, ν - outer normal to Ω_1, g - gravity, σ - surface tension, $\mathbb{P}_\Gamma$ - projection to tangential plane, μ_j - dynamic viscosity, σ_0 - reference surface tension, $c_{\Gamma,0}$ - reference concentration, R - ideal gas constant, T_a - absolute temperature , $[|.|]$ - jump of quantity across Γ

Convection-Diffusion Equations

Insoluble surfactant

Surfactant concentration on the surface

$$\dot{c}_\Gamma + c_\Gamma \nabla_\Gamma \cdot \mathbf{w} + \nabla_\Gamma \cdot [c_\Gamma \mathbb{P}_\Gamma(\mathbf{u} - \mathbf{w})] = D_\Gamma \Delta_\Gamma c_\Gamma \qquad \text{on } \Gamma(t)$$

$+$ initial conditions

c_Γ - surf. surfactant concentration, $\mathbf{u}$ - velocity, $\mathbf{w}$ - surf. velocity ,D_Γ - surf. diffusion coefficient, $\mathbb{P}_\Gamma$ - projection to tangential plane,

Convection-Diffusion Equations

Soluble surfactant

Surfactant concentration on the surface

$$\dot{c}_\Gamma + c_\Gamma \nabla_\Gamma \cdot \mathbf{w} + \nabla_\Gamma \cdot [c_\Gamma \mathbb{P}_\Gamma(\mathbf{u} - \mathbf{w})] = D_\Gamma \Delta_\Gamma c_\Gamma + S(c_\Gamma, c_1, c_2) \qquad \text{on } \Gamma(t)$$

+ initial conditions

Surfactant concentration in the phases

$$\frac{\partial c_j}{\partial t} + (\mathbf{u} \cdot \nabla) c_j = D_j \Delta c_j \qquad \text{in } \Omega_j(t)$$

$$[|D(\nu \cdot \nabla c)|] = -S(c_\Gamma, c_1, c_2) \qquad \text{on } \Gamma(t)$$

+ initial and appropriate boundary conditions

c_Γ - surf. surfactant concentration, $\mathbf{u}$ - velocity, $\mathbf{w}$ - surf. velocity ,D_Γ - surf. diffusion coefficient, $\mathbb{P}_\Gamma$ - projection to tangential plane, c_j - surfactant concentration, D_j - diffusion coefficient,

Convection-Diffusion Equations

Soluble surfactant

Surfactant concentration on the surface

$$\dot{c}_\Gamma + c_\Gamma \nabla_\Gamma \cdot \mathbf{w} + \nabla_\Gamma \cdot [c_\Gamma \mathbb{P}_\Gamma (\mathbf{u} - \mathbf{w})] = D_\Gamma \Delta_\Gamma c_\Gamma + S(c_\Gamma, c_1, c_2) \qquad \text{on } \Gamma(t)$$

$+$ initial conditions

Surfactant concentration in the phases

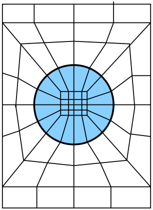
$$\begin{aligned} \frac{\partial c_j}{\partial t} + (\mathbf{u} \cdot \nabla) c_j &= D_j \Delta c_j && \text{in } \Omega_j(t) \\ [|D(\nu \cdot \nabla c)|] &= -S(c_\Gamma, c_1, c_2) && \text{on } \Gamma(t) \end{aligned}$$

$+$ initial and appropriate boundary conditions

$$\begin{aligned} S(c_\Gamma, c_1, c_2) &= (k_{a,1} c_1 + k_{a,2} c_2) \left(1 - \frac{c_\Gamma}{c_{\Gamma,\infty}}\right) - (k_{d,1} + k_{d,2})\, c_\Gamma && \text{(Langmuir)} \\ S(c_\Gamma, c_1, c_2) &= k_{a,1} c_1 + k_{a,2} c_2 - (k_{d,1} + k_{d,2})\, c_\Gamma && \text{(Henry)} \end{aligned}$$

c_Γ - surf. surfactant concentration, $\mathbf{u}$ - velocity, $\mathbf{w}$ - surf. velocity ,D_Γ - surf. diffusion coefficient, $\mathbb{P}_\Gamma$ - projection to tangential plane,
c_j - surfactant concentration, D_j - diffusion coefficient, $k_{a,j}$, $k_{d,j}$ - adsorption/desorption coefficients,
Γ_∞ - maximum surface surfactant concentration

Interface tracking method



Arbitrary Lagrangian Eulerian approach (our choice)

- Interface and boundaries move with the fluid (Lagrangian manner)
- Inner points can be displaced arbitrarily

ALE form of the NSE and Bulk-CDE

$$\frac{\partial \mathbf{u}}{\partial t}\Big|_{\hat{\Omega}} + (\mathbf{u} - w) \cdot \nabla \mathbf{u} - \nabla \cdot \mathbb{S}(\mathbf{u}, p) = f$$

$$\frac{\partial c}{\partial t}\Big|_{\hat{\Omega}} + (\mathbf{u} - w) \cdot \nabla c = D \Delta c$$

Advantages

- jump in material properties can be handled easily
- surface force can be incorporated more precisely
- excellent mass conservation can be achieved
- spurious velocities can be suppressed with appropriate choice of finite elements

- S. Ganesan, L. Tobiska: *"Arbitrary Lagrangian-Eulerian method for computation of two-phase flows with soluble surfactant"*, J. Comp. Phy.,(2012)
- S. Ganesan, L. Tobiska: *"A coupled arbitrary Lagrangian-Eulerian and Lagrangian method for computation of free surface flows with insoluble surfactants"*, J. Comp. Phy.,(2009)

Oscillating Droplet

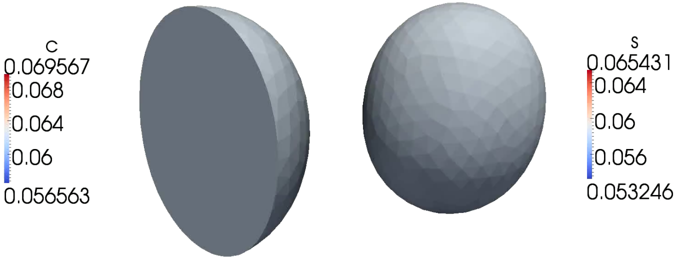


Table : Initial surfactant concentrations

Case	$C(0)$	$c_\Gamma(0)$	Total mass
clean	–	–	–
i	3.0391×10^{-2}	2.9495×10^{-2}	0.5
ii	6.2170×10^{-2}	5.8531×10^{-2}	1
iii	1.3013×10^{-1}	1.1515×10^{-1}	2

Oscillating Droplet

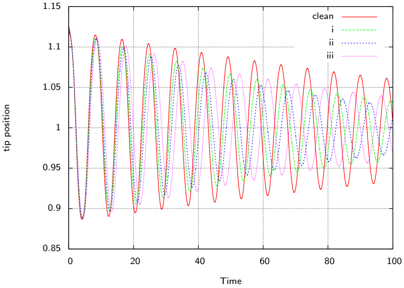
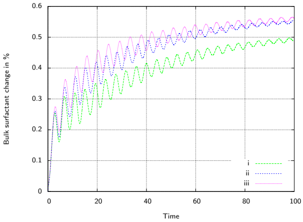


Figure : Tip postion of the oscillating bubble.



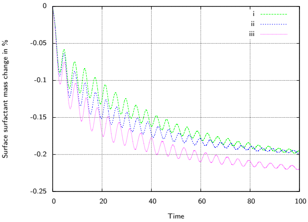
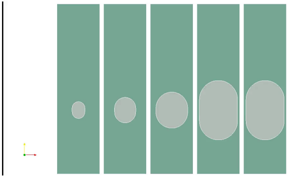
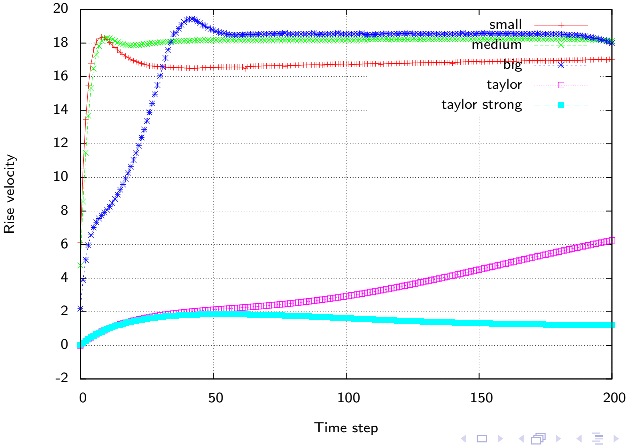


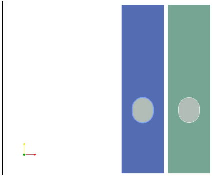
Figure : Mass of the bulk surfactant (left) and mass of the surface surfactant (right).

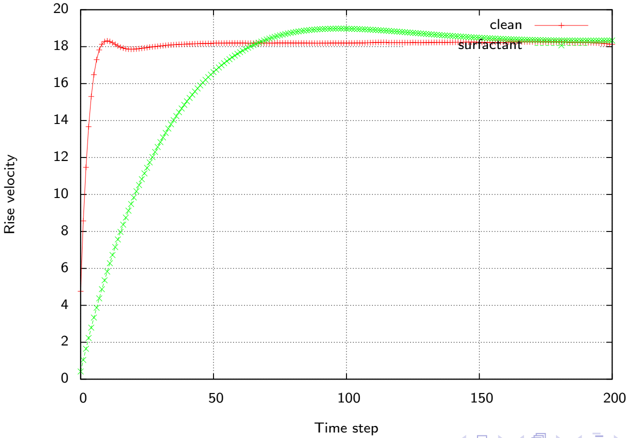
Rising Drops and Taylor Bubbles



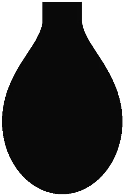


Rising Drops and Taylor Bubbles

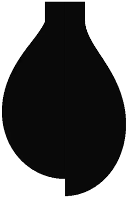




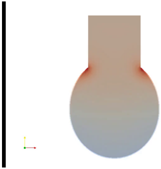
Pending Drop



Growing pending drop



Growing pending drop - comparsion



Oscillating pending drop

Thank you for your attention and support.