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8th June 2025
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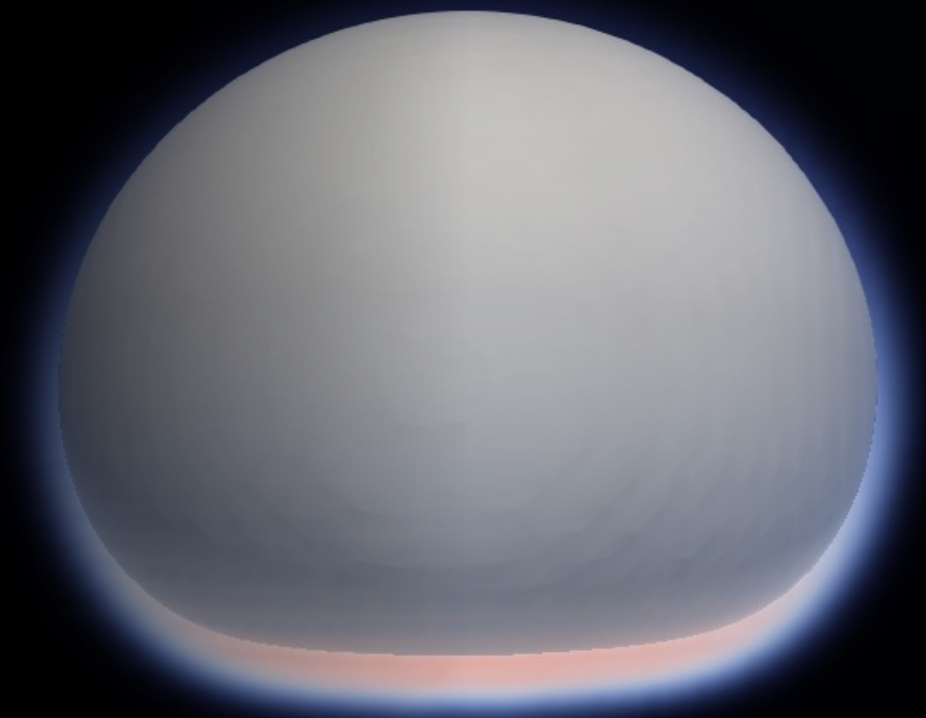

Surfactant Transport at finite Péclet numbers

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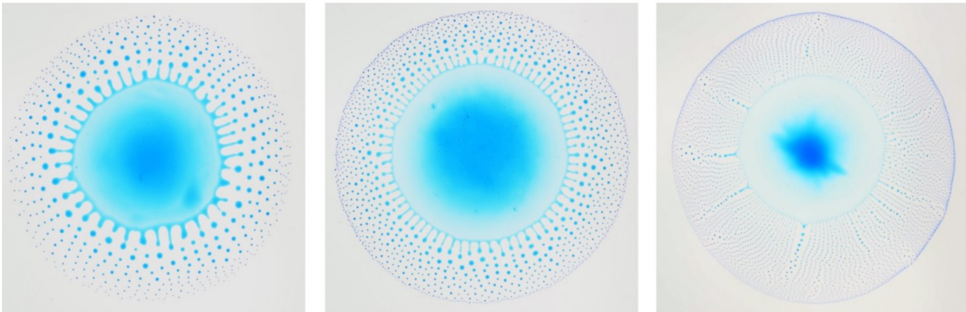
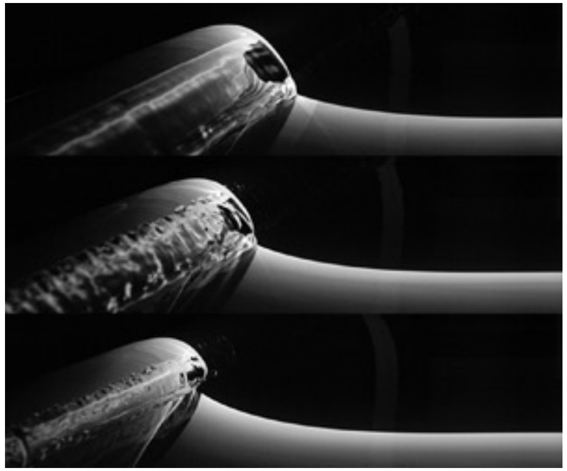
Motivation: Surfactant laded flows and Marangoni effect

Tears of wine (CCL)



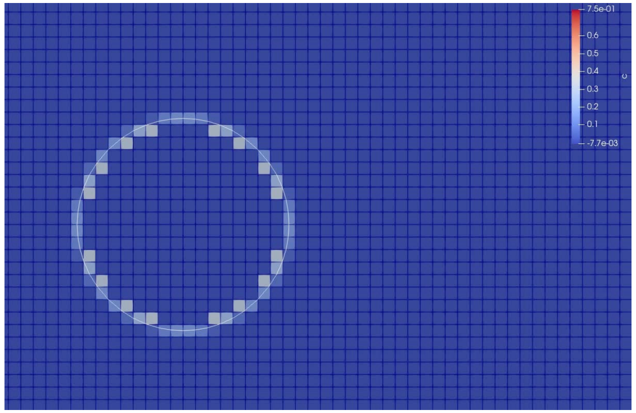
Marangoni Bursting - Durey et. al. (2018)



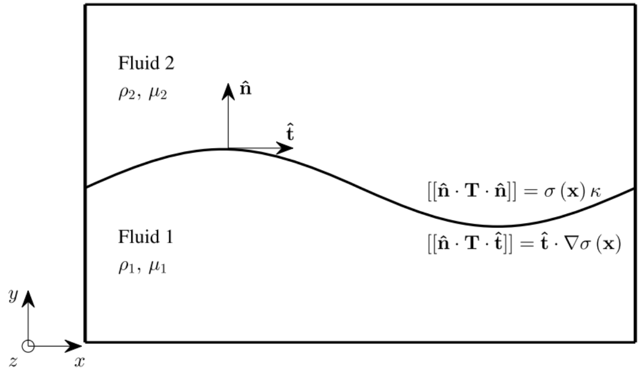
The effects of surfactants on plunging breakers (Erinin. et. al. 2023)

Marangoni Effect due to insoluble surfactants

$$\frac{\partial \Gamma}{\partial t} + \nabla_s \cdot (\Gamma \mathbf{u}_s) + \Gamma(\nabla_s \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{n}) = D\nabla_s^2 \Gamma$$



Unsuccessful attempt with VoF



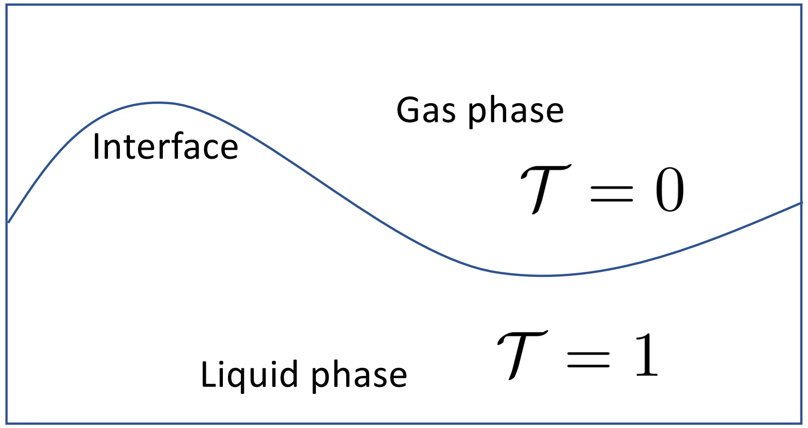
Seric, I., Afkhami, S., & Kondic, L. (2018). Direct numerical simulation of variable surface tension flows using a volume-of-fluid method. *Journal of Computational Physics*, *352*, 615-636.

$$\partial_t \boldsymbol{u} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\boldsymbol{u}) = \frac{1}{\rho}\left[-\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot (\mu(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T))\right] + \frac{\gamma}{\rho}\kappa\delta_s \boldsymbol{n} + \delta_m \nabla_s \gamma$$

Numerical Framework

Navier-Stokes equations and two-phase flows

$$\partial_t \boldsymbol{u} + \boldsymbol{\nabla}\cdot(\boldsymbol{u}\boldsymbol{u}) = \frac{1}{\rho}\left[-\boldsymbol{\nabla} p + \boldsymbol{\nabla}\cdot\left(\mu(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T)\right)\right] + \frac{\gamma}{\rho}\kappa\delta_s \boldsymbol{n},$$
$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0,$$
$$\frac{\partial \mathcal{T}}{\partial t} + \boldsymbol{\nabla}\cdot(\mathcal{T}\mathbf{u}) = 0.$$



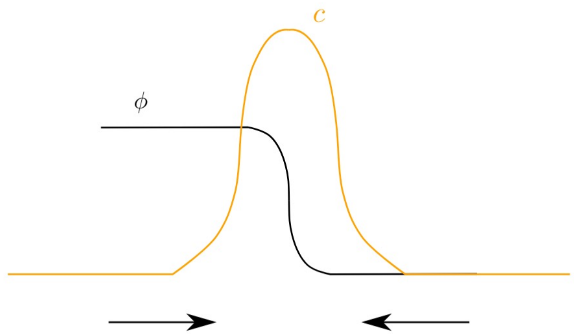
Velocity, pressure, interface

Volume of fluid (VOF) method to capture the interface

$$\frac{\partial \Gamma}{\partial t} + \nabla_s\cdot(\Gamma\mathbf{u}_s) + \Gamma(\nabla_s\cdot\mathbf{n})(\mathbf{u}\cdot\mathbf{n}) = D_s\nabla_s^2\Gamma$$ Surfactant Transport equation, Scriven (1960), Stone (1990)

$$\frac{\partial c}{\partial t} + \nabla\cdot(uc) = \nabla\cdot\left[D_s\left\{\nabla c - \frac{2(0.5-\phi)\vec{n}c}{\epsilon}\right\}\right]$$ Volumetric surfactant concentration

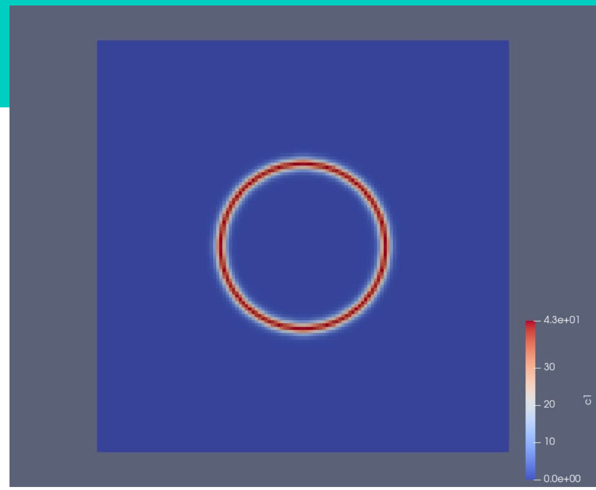
$$\phi = \frac{1}{2\epsilon}\tanh\left(\text{Signed Distance}(\mathcal{T})\right)$$ Phase-Field



Suhas Jain, A model for transport of interface-confined scalars and insoluble surfactants in two-phase flows, Journal of Computational Physics, 515, 113277

Palas Kumar Farsoiya, Stéphane Popinet, Howard A. Stone, Luc Deike, A coupled Volume of Fluid - Phase Field method for direct numerical simulation of insoluble surfactant-laden interfacial flows and application to rising bubbles, Physical Review Fluids, Vol 9, 094004, (2024).

Test Case I – Expansion term



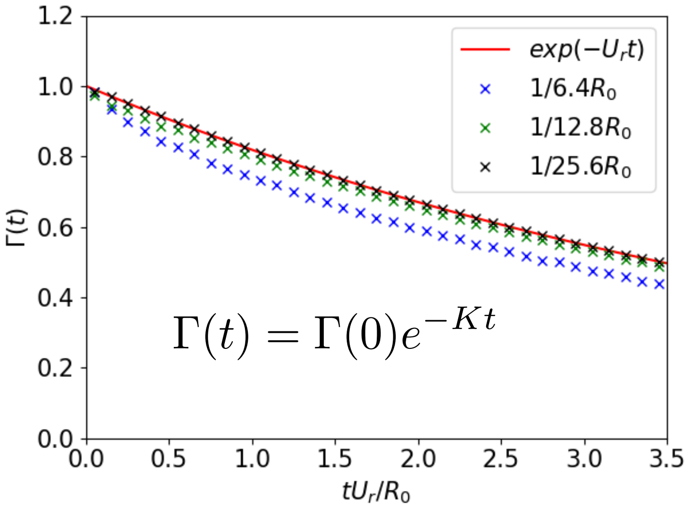
$tU_r/R_0 = 0$ $\quad$ $tU_r/R_0 = 3.5$

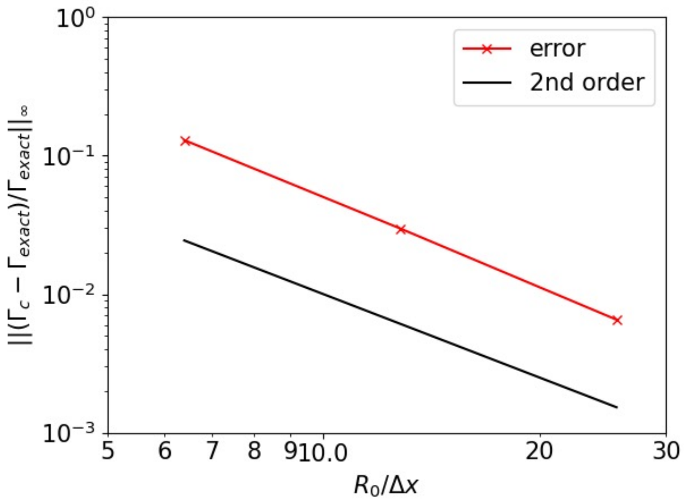
Stone (1990) and Atasi et. al. (2018)

$$\frac{\partial \Gamma}{\partial t} + \nabla_s \cdot (\Gamma \mathbf{u}_s) + \Gamma(\nabla_s \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{n}) = D_s \nabla_s^2 \Gamma$$

$$\frac{\partial \Gamma}{\partial t} + \Gamma(\nabla_s \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{n}) = 0 \qquad \mathbf{u}(r, \theta, \phi) = U_r r \hat{e}_r$$

$$\frac{d\,\Gamma}{dt} + \Gamma \frac{1}{r} U_r r = 0$$





Test Case II - Advection and Diffusion term

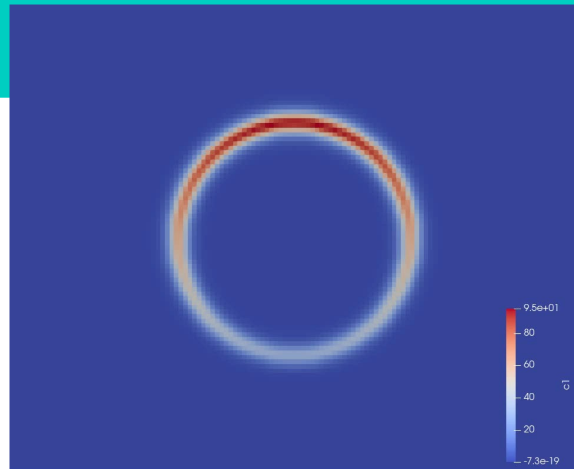
Atasi et. al. (2018)

$$\frac{\partial \Gamma}{\partial t} + \nabla_s \cdot (\Gamma \mathbf{u}_s) + \Gamma(\nabla_s \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{n}) = D_s \nabla_s^2 \Gamma$$

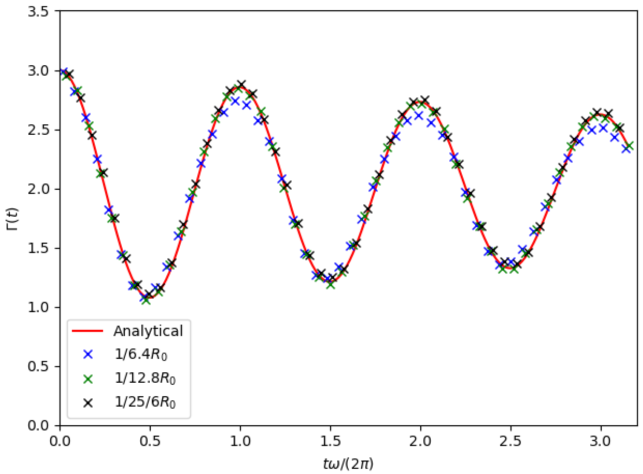
Analytical

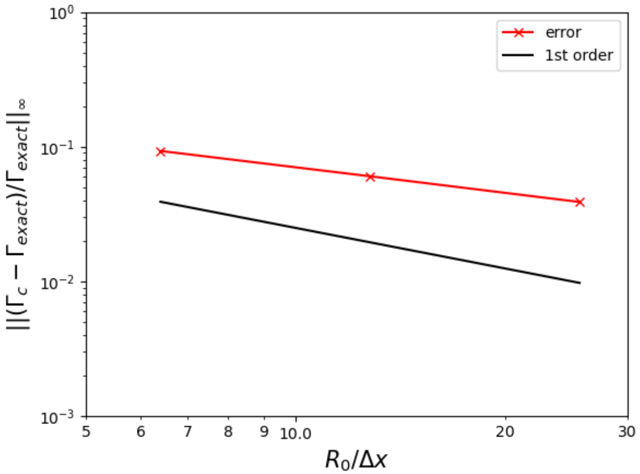
$$\Gamma(\theta, 0) = 2 + \sin\theta$$

$$\Gamma(\theta, t) = 2 + \sin(\omega t + \theta) e^{-D/R^2 t}$$

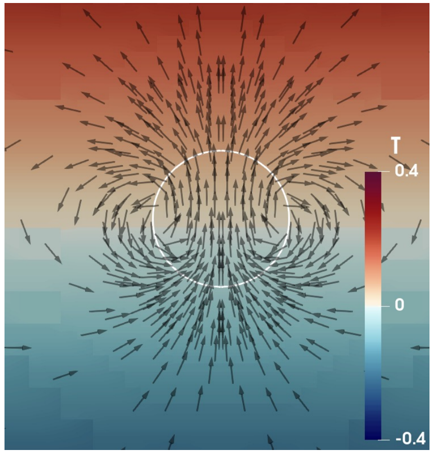


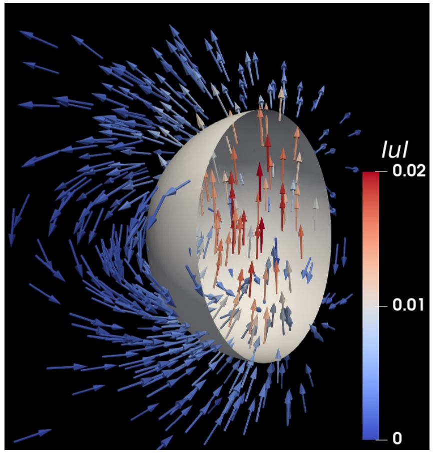
$t\omega/(2\pi) = 0$ $\qquad$ $t\omega/(2\pi) = 3.2$





Droplet migration in thermal gradient



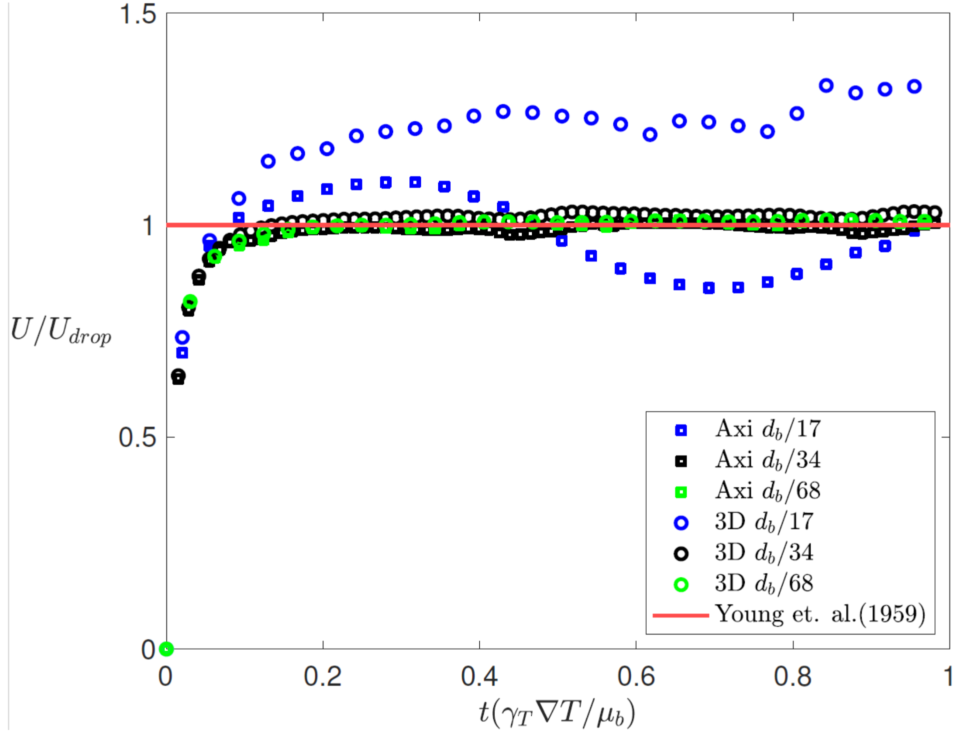


$$Re = 0.066,\ Ca = 0.066$$

Increasing temperature

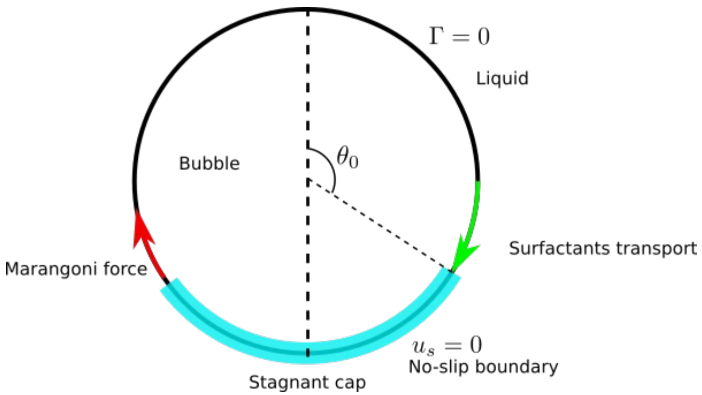
$$U_{drop} = \frac{-2}{6 + 9\mu_{drop}/\mu_{bulk}} \frac{\gamma_T R \nabla T}{\mu_{bulk}}$$

Young et. al. (1959)



$$\partial_t \boldsymbol{u} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\boldsymbol{u}) = \frac{1}{\rho}\left[-\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot (\mu(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T))\right] + \frac{\gamma}{\rho}\kappa\delta_s \boldsymbol{n} + \delta_m \nabla_s \gamma$$

Revisiting the Effect of surfactants on a rising bubble using DNS



Contaminated rising bubble at steady state

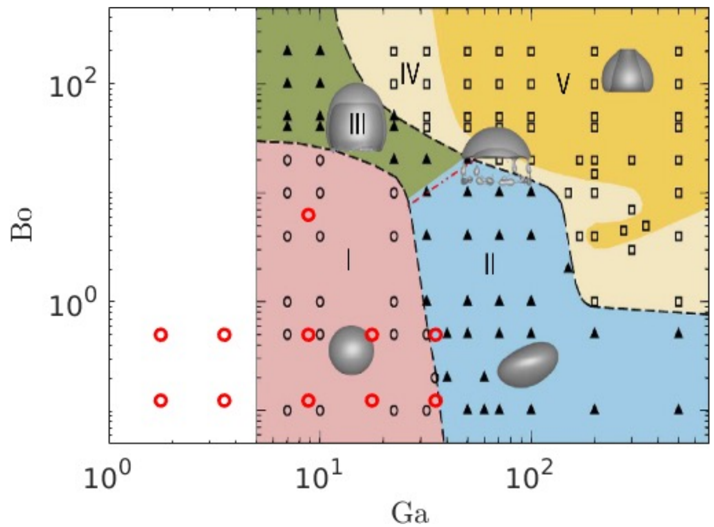
$$Ga = \frac{\rho_l d_b \sqrt{g d_b}}{\mu_l} \qquad Bo = Eo = \frac{\rho_l g d_b^2}{\gamma_0}$$

Isotherm/Equation of State

$$\gamma(x,t) = \gamma_0 \left(1 - \beta \frac{\Gamma(x,t)}{\Gamma_0}\right)$$

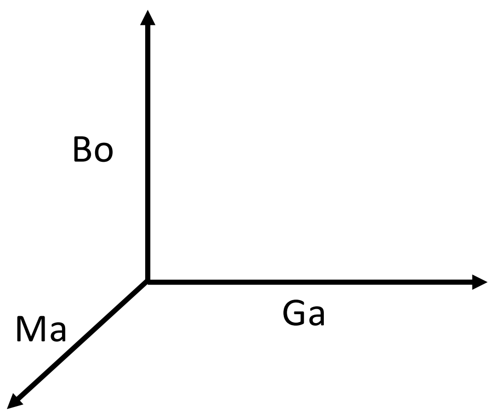
$$Ma = \frac{\beta \gamma_0}{\mu_l \sqrt{g d_b}}$$

$$Re = \frac{\rho_l U_b d_b}{\mu_l} = f(Ga, Bo, Ma)$$



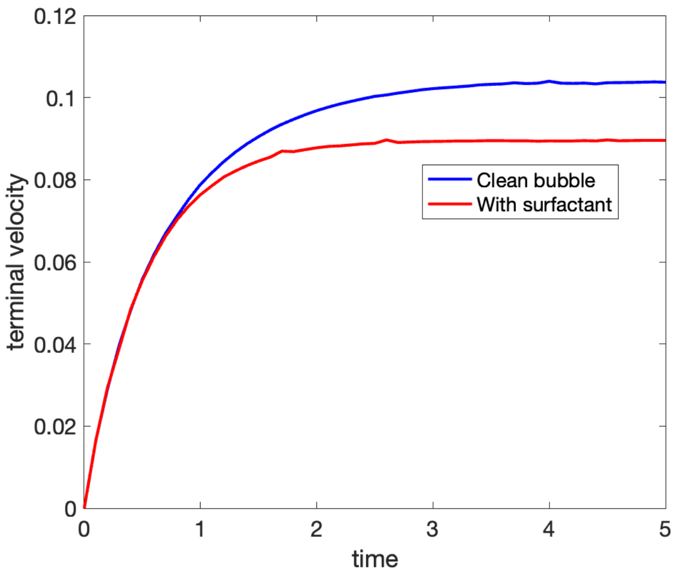
Tripathi, Manoj Kumar, Kirti Chandra Sahu, and Rama Govindarajan. "Dynamics of an initially spherical bubble rising in quiescent liquid." *Nature communications* 6.1 (2015): 6268.

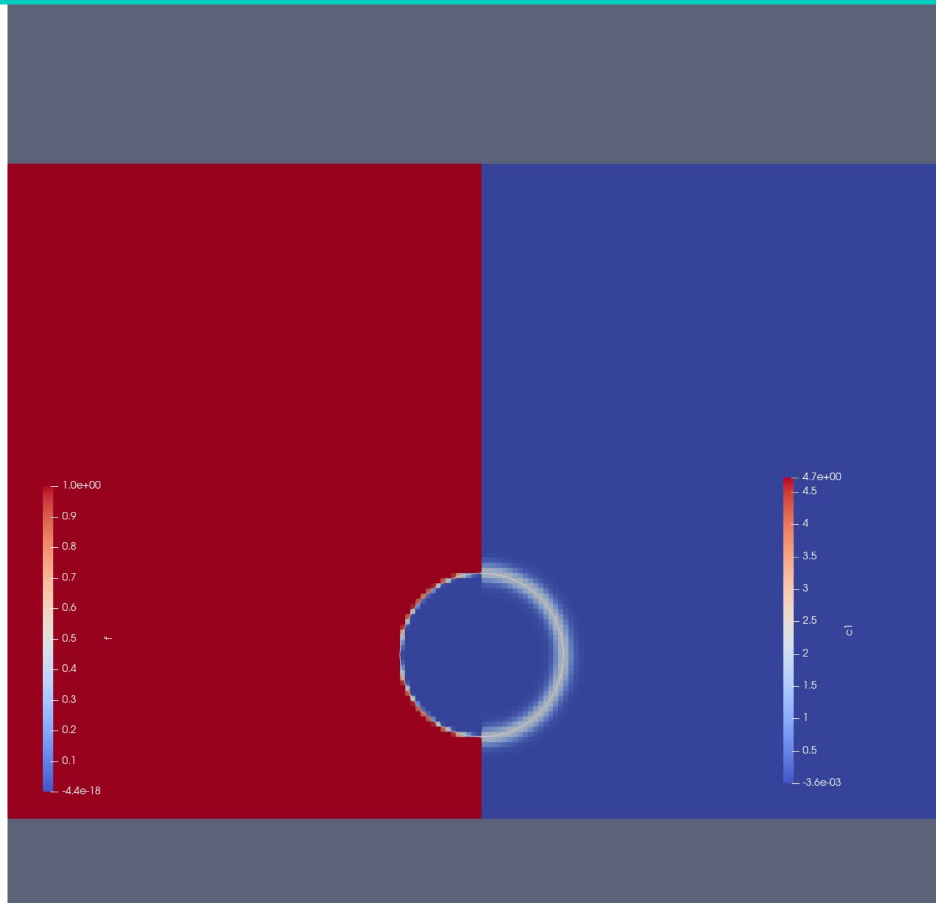
Present Study



Revisiting the Effect of surfactants on a rising bubble using DNS

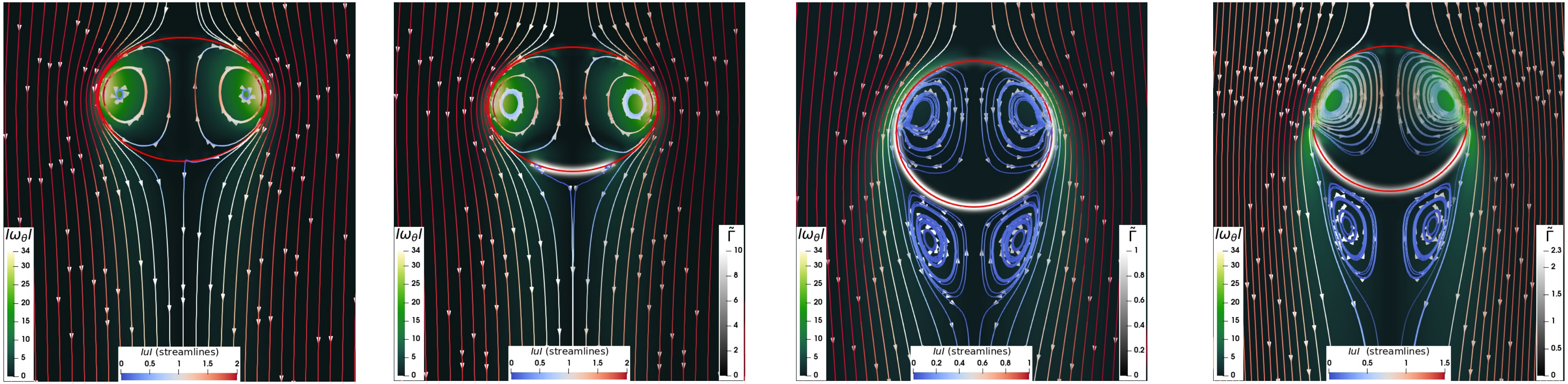
$$\sigma(x,t) = \sigma_0 \left(1 - \beta \frac{\Gamma(x,t)}{\Gamma_0}\right)$$





Surfactant-laden axisymmetric rising bubble

$Ga = 100, \quad Bo = 0.5$



$Ma = 0$

Clean

$Re = 200$

$Ma = 0.1$

$Re = 200$

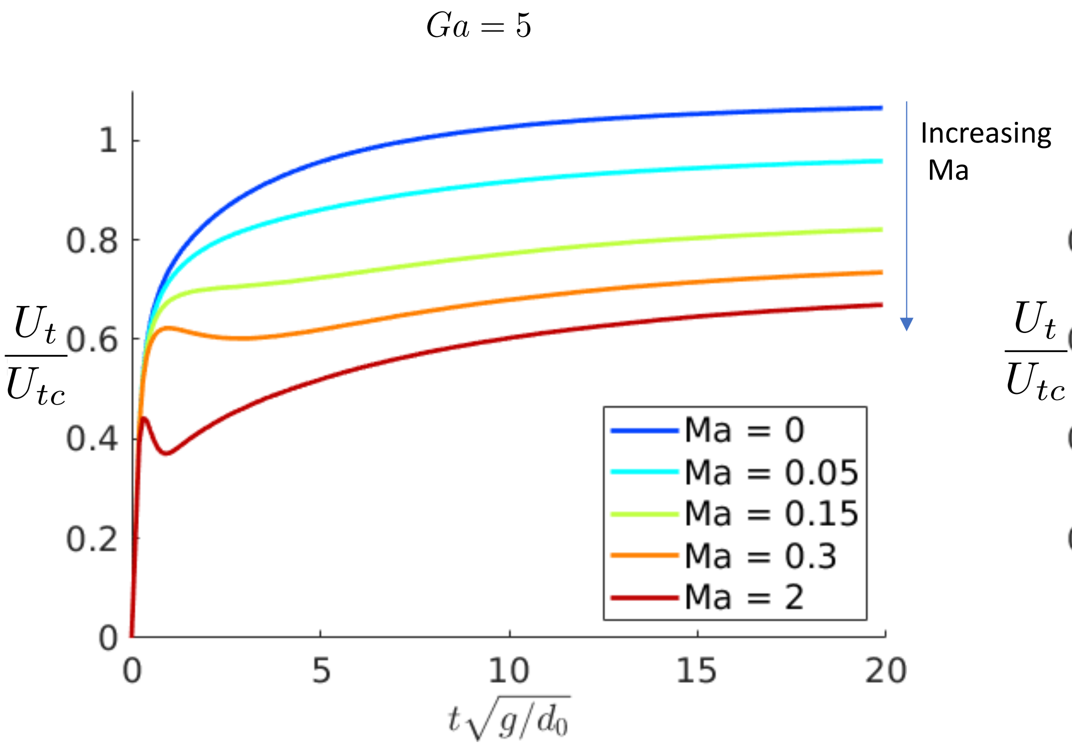
$Ma = 1$

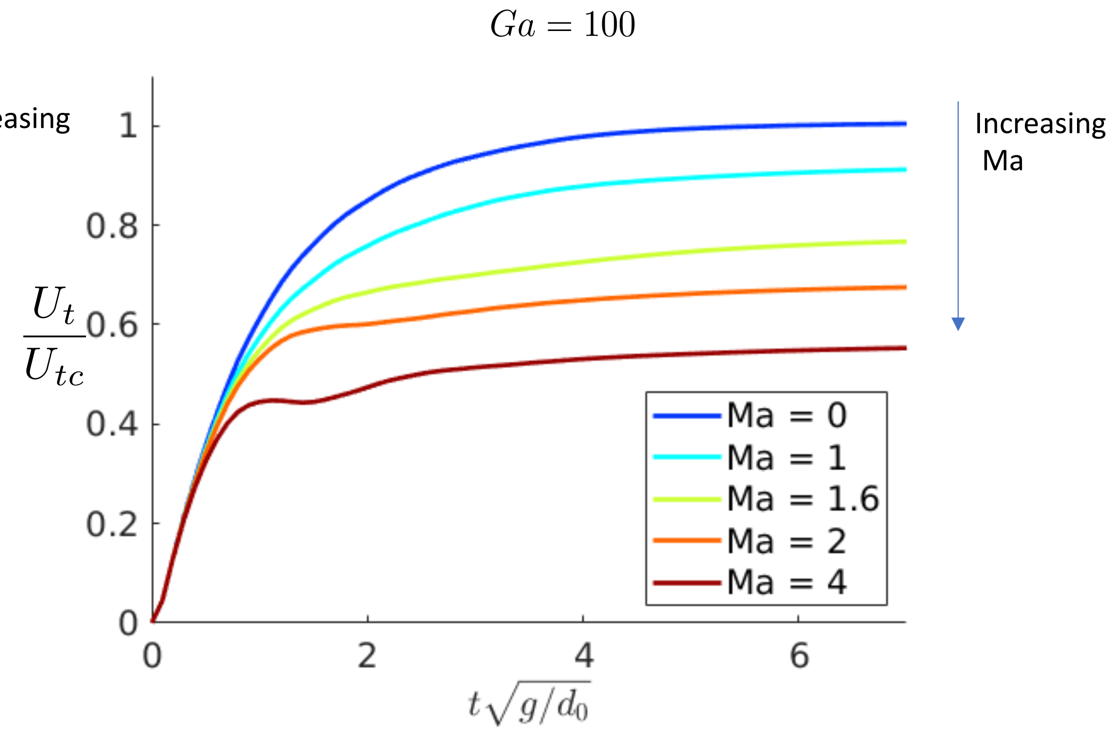
$Re = 150$

$Ma = 10$

$Re = 100$

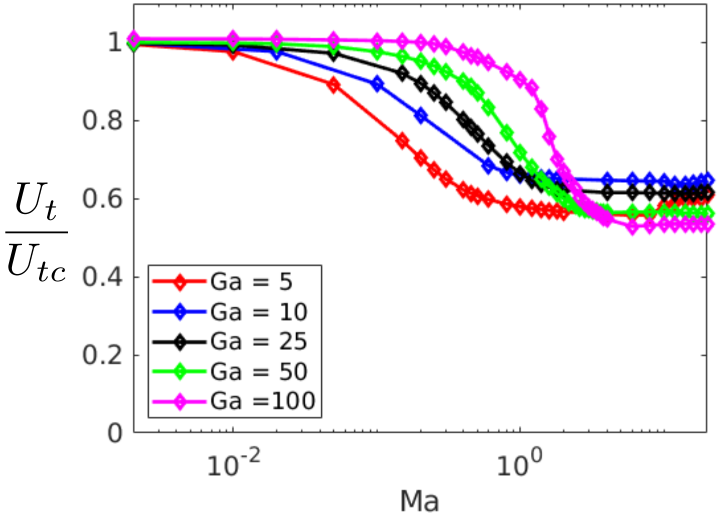
Reduction in rise velocity w.r.t Ma at different Ga

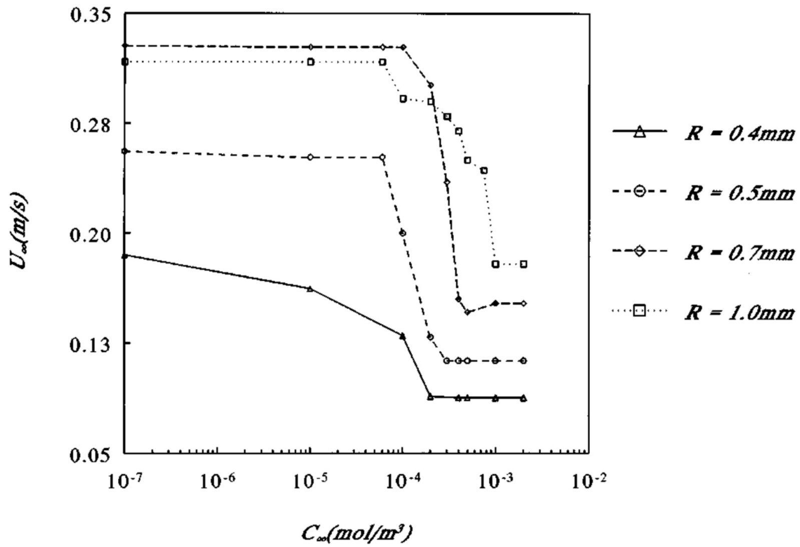




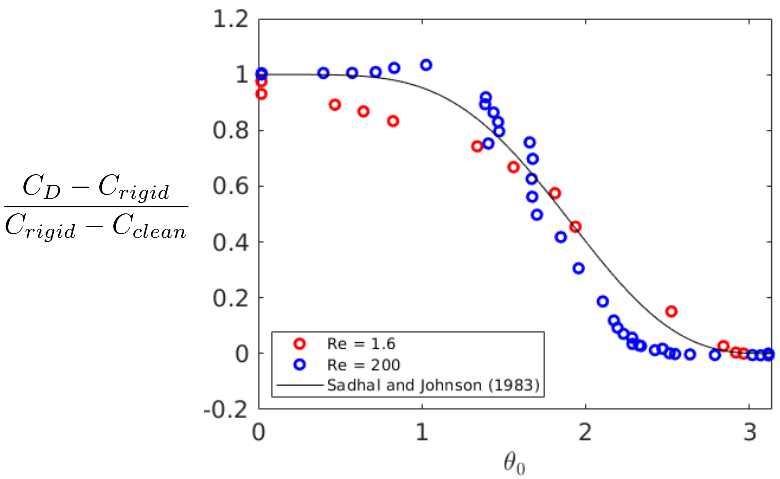
U_{tc} Terminal velocity of Clean bubble

Effect of Marangoni number and stagnant cap

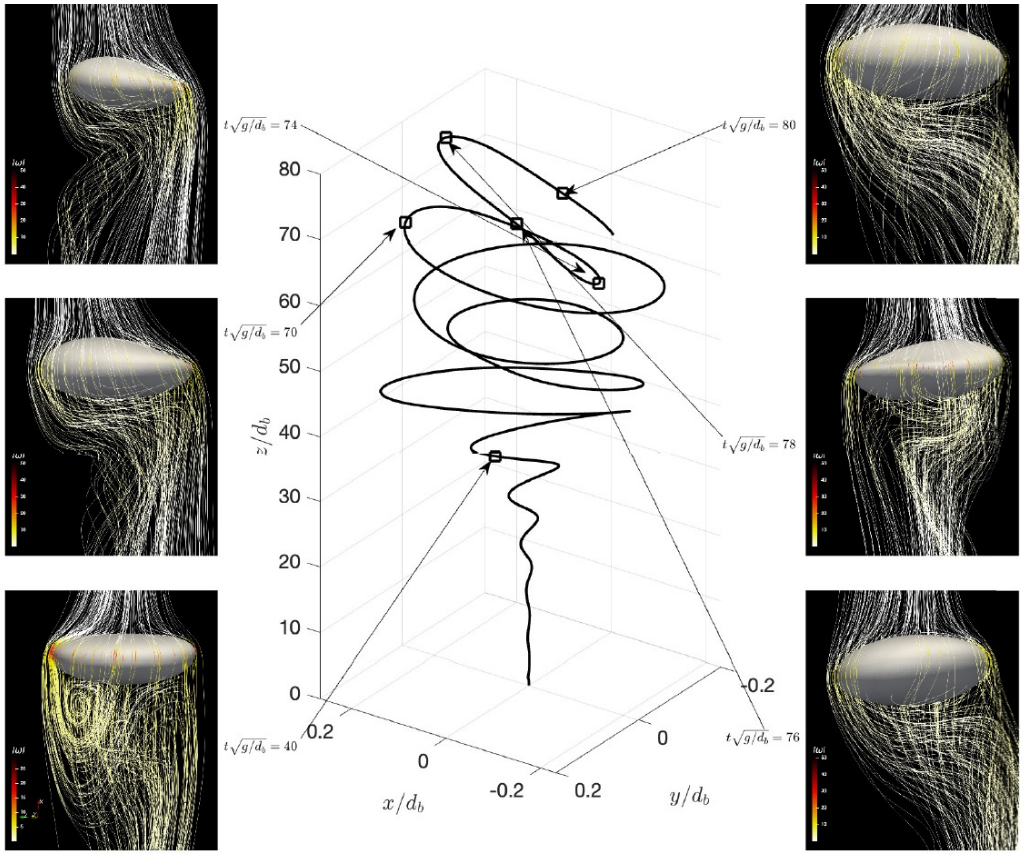




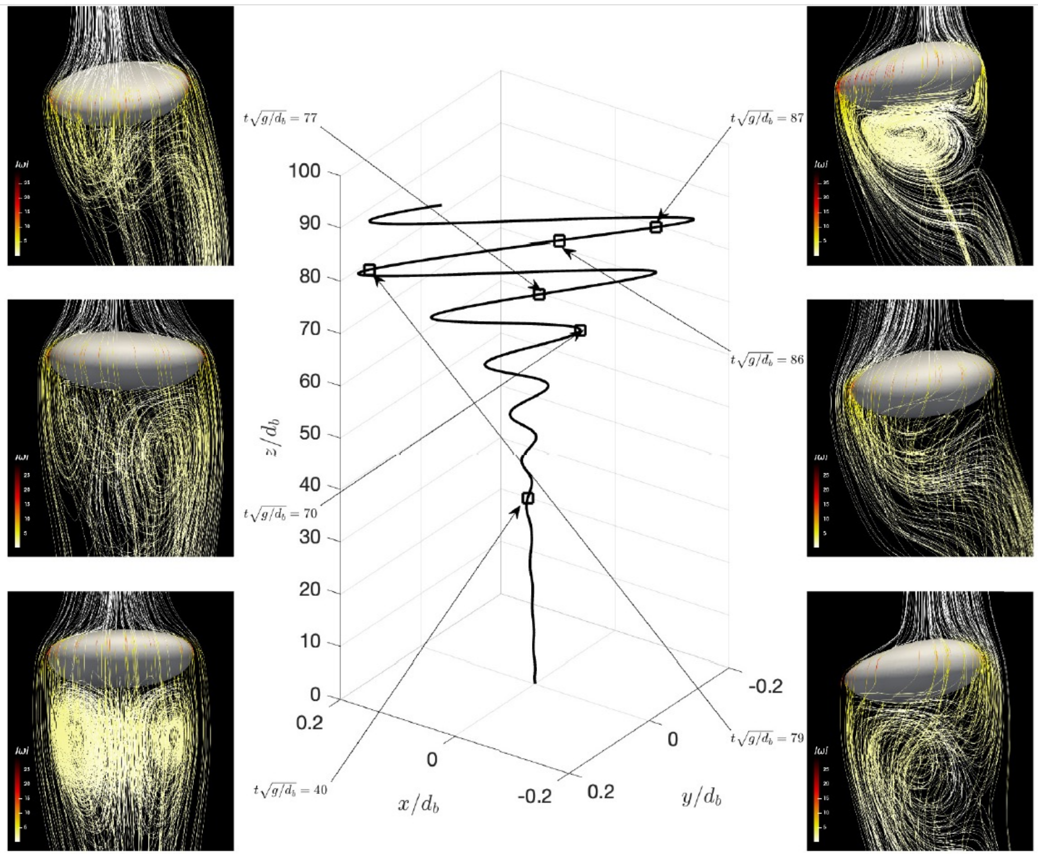
Experiments by Fdhila and Duineveld (1996)



Trajectory of surfactant-laden 3D rising bubble

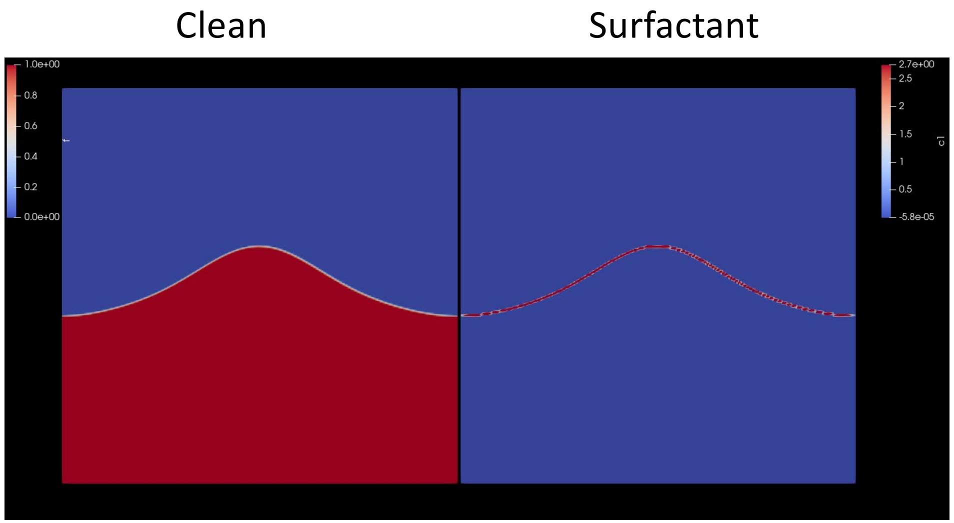


Helical trajectory of clean bubble



Zigzag trajectory of surfactant-laden bubble

Surfactant-laden waves



Thanks