IMPERIAL

Department of
Chemical Engineering

Direct numerical simulations of Multiphase Flows in Stirred Vessels and Static Mixers

Omar Matar
10/10/2024

Multiphase flows
Challenges

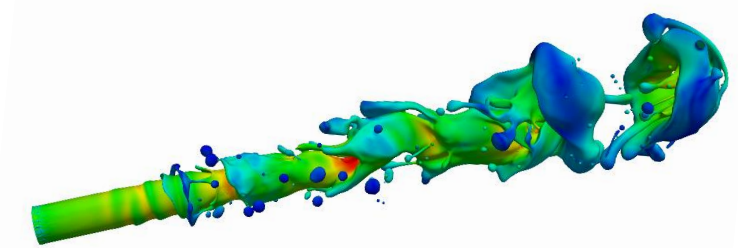
Multiphase flows are discontinuous

- Phase-interface extremely thin and exhibits a singular surface tension force
- Fluid properties jump across the interface

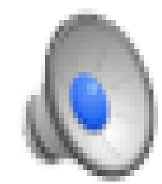
Multiphase flows are multi-scale

- From microscopic droplets to meters (oceanic flows)
- Complex topology changes
- Turbulence (atomisation)

Multi-scale: oceanic flows



Discontinuous: Atomisation



Multi-physics: dirty interfaces

Multiphase flow are multi-physics

- **Surfactant-laden** interfaces featuring Marangoni stresses (dirty interfaces)
- Non-isothermal, phase change

Numerical simulations facilitate isolation of mechanisms

Multiphase Flows
Governing Equations

- N-S equations:

$C_s = 0.2$, Smagorinsky-Lilly coefficient
Large Eddy Simulation

$$\nabla \cdot \widetilde{\boldsymbol{u}} = 0,$$

$$\tilde{\rho}\left(\frac{\partial \widetilde{\boldsymbol{u}}}{\partial \tilde{t}} + \widetilde{\boldsymbol{u}} \cdot \nabla \widetilde{\boldsymbol{u}}\right) = -\nabla \tilde{p} + \frac{1}{Re} \nabla \cdot \tilde{\mu}\left(\nabla \widetilde{\boldsymbol{u}} + \nabla \widetilde{\boldsymbol{u}}^T\right) - \nabla \cdot \left(\tilde{\rho} C_s^2 \widetilde{\Delta}^2 |\tilde{s}|\right)\left(\nabla \widetilde{\boldsymbol{u}} + \nabla \widetilde{\boldsymbol{u}}^T\right) - \frac{1}{Fr} \tilde{\rho} \widetilde{\boldsymbol{g}} + \widetilde{\boldsymbol{F}}_{fsi}$$
$$+ \frac{1}{We}\left(\int_{\tilde{A}_e} \tilde{\sigma} \tilde{\kappa} \boldsymbol{n} + \nabla_s \tilde{\sigma}\right) \delta_f\left(\widetilde{\boldsymbol{x}} - \widetilde{\boldsymbol{x}}_f\right) d\tilde{A}_e\right),$$

$\Delta \equiv \min(\Delta x, \Delta y, \Delta z)$

Solid-fluid interaction force

Normal component: mean interfacial tension

Tangential component: Marangoni stresses

- *Interface behaviors*

Hybrid front-tracking/level-set method[1]

- *Rotating impeller*

Direct-Forcing method[2]

[1] Shin, S., Chergui, J., Juric, D., Kahouadji, L., Matar, O. K., & Craster, R. V. (2018). A hybrid interface tracking–level set technique for multiphase flow with soluble surfactant. *Journal of Computational Physics*, 359, 409-435.

[2] Fadlun, E. A., Verzicco, R., Orlandi, P., & Mohd-Yusof, J. (2000). Combined immersed-boundary finite-difference methods for three-dimensional complex flow simulations. *Journal of computational physics*, *161*(1), 35-60.

Multiphase Flows
Governing Equations

- Surfactant transport:

Bulk: $$\frac{\partial \tilde{C}}{\partial t} + \tilde{\boldsymbol{u}} \cdot \nabla \tilde{C} = \frac{1}{Pe_b} \nabla^2 \tilde{C},$$

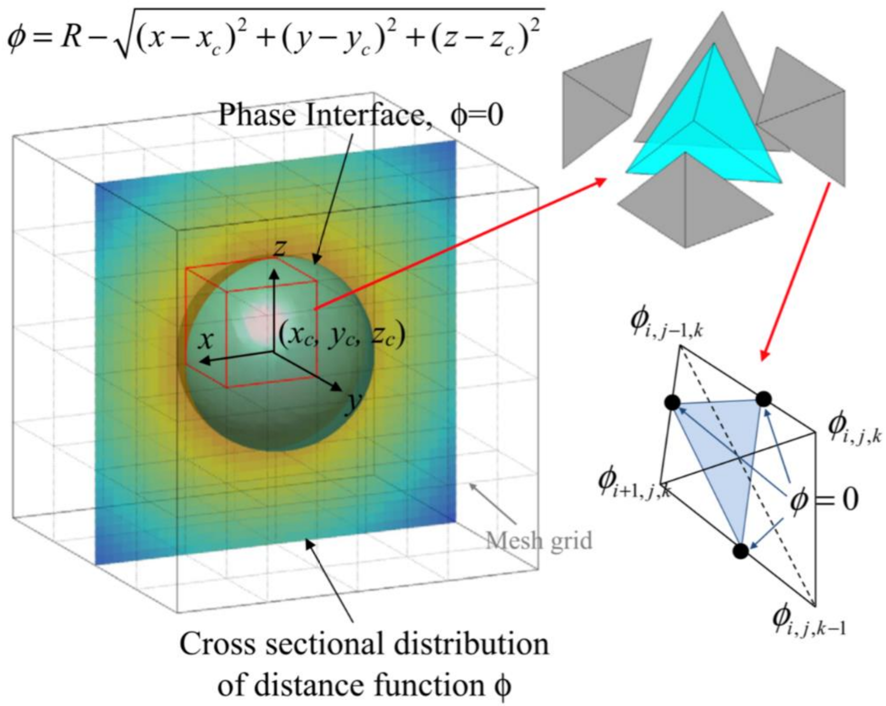
Interface: $$\frac{\partial \tilde{\Gamma}}{\partial t} + \nabla_s \cdot \left(\tilde{\Gamma} \tilde{\boldsymbol{u}}_t\right) = \frac{1}{Pe_s} \nabla_s^2 \tilde{\Gamma} + \tilde{J},$$

Ad/des flux: $$\tilde{J}_{a/d} = Bi\left[k \tilde{C}_0 \left(1 - \tilde{\Gamma}\right) - \tilde{\Gamma}\right],$$

Diffusive flux : $$\tilde{J}_{diff} = -\frac{1}{Pe_b h} \boldsymbol{n} \cdot \nabla \tilde{C}|_{sub}$$

Langmuir relation: $$\tilde{\sigma} = \max[0.05, 1 + \beta_s \ln\left(1 - \tilde{\Gamma}\right)]\,.$$

Multiphase Flows
Numerical Method



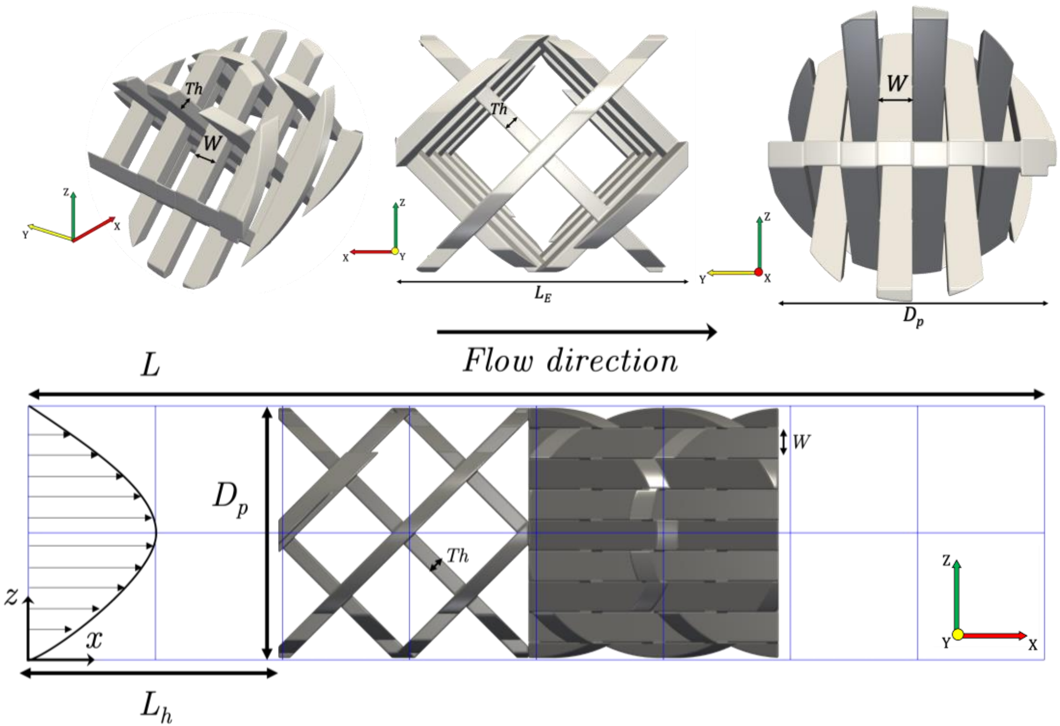
*Hybrid **front-tracking/level-set** methods*

- Accurate calculation of surface tension forces
- It can handle complex topological changes
- Mass conservation
- Lagrangian interface tracking

Imperial College London PREMIERE memphis multiphase EPSRC Engineering and Physical Sciences Research Council




Static Mixers
Geometry



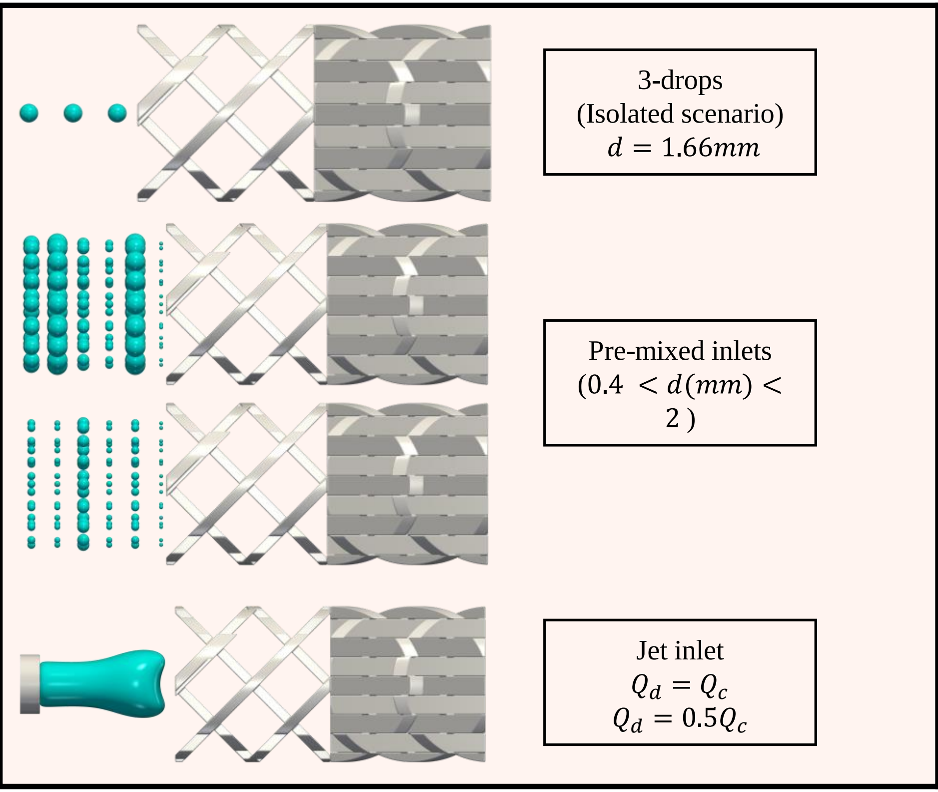
Liu et al. (2005) and *Rama Rao et al. (2007)* specifications

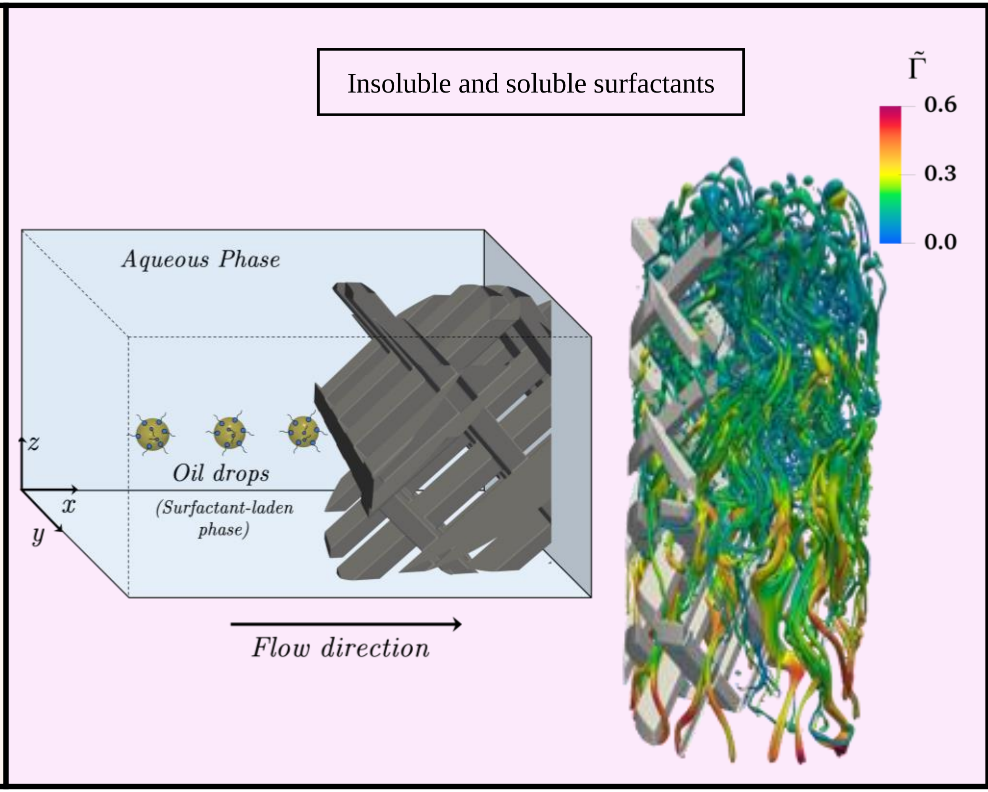
Feature		
Pipe diameter D_P (m)	0.01575	
Number of crossbars	8	
Aspect ratio L_E/D_P	1	
Entry length L_h (m)	0.01575	
Number of elements n_E	2	
Bar thickness Th (m)	0.001	
Bar width W (m)	0.0019	
Length L (m)	0.064	
	Subdomains	Cells per subdomain
Grid details	$12 \times 6 \times 6$	$128 \times 64 \times 64$

	Continuous	Dispersed
Density ρ (kg/m^3)	1364	960
Viscosity μ $(Pa \cdot s)$	0.615	0.0984
Surface tension σ (N/m)	0.036	
Flow rate Q (m^3/s)	9.0e-6	
Re	1.63	

Static Mixers

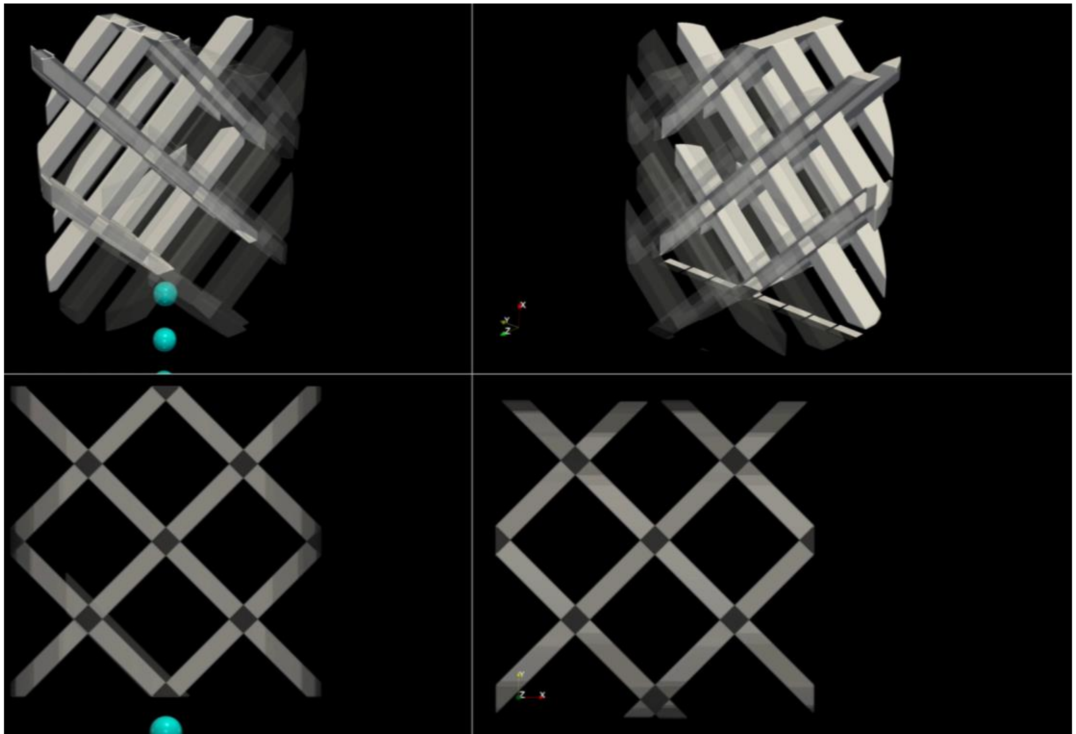
Case Studies





Static Mixers

Two-stage Breakup

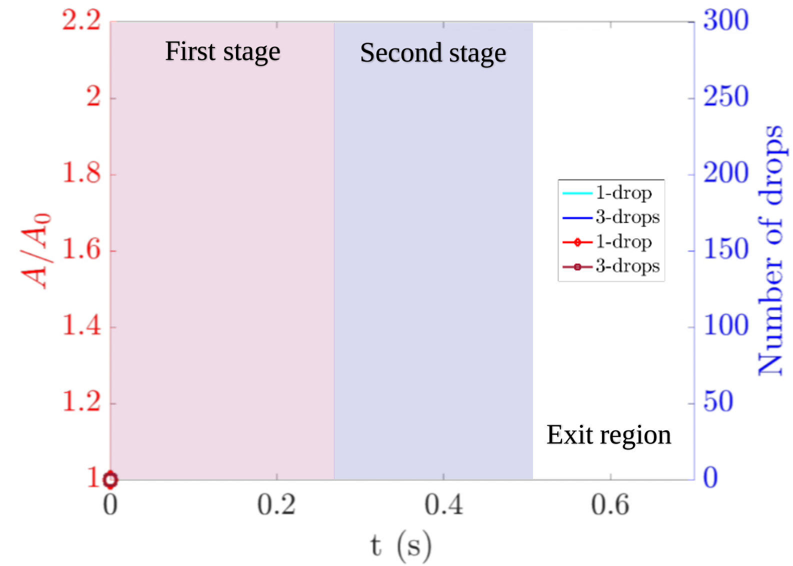


3-drops

Contents lists available at ScienceDirect
Chemical Engineering Journal
journal homepage: www.elsevier.com/locate/cej

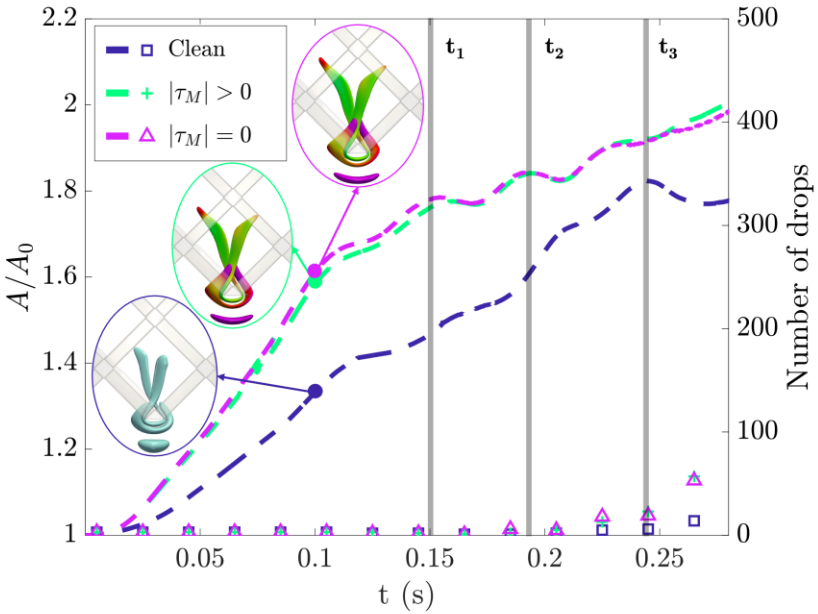
Direct numerical simulations of liquid–liquid dispersions in a SMX mixer under different inlet conditions

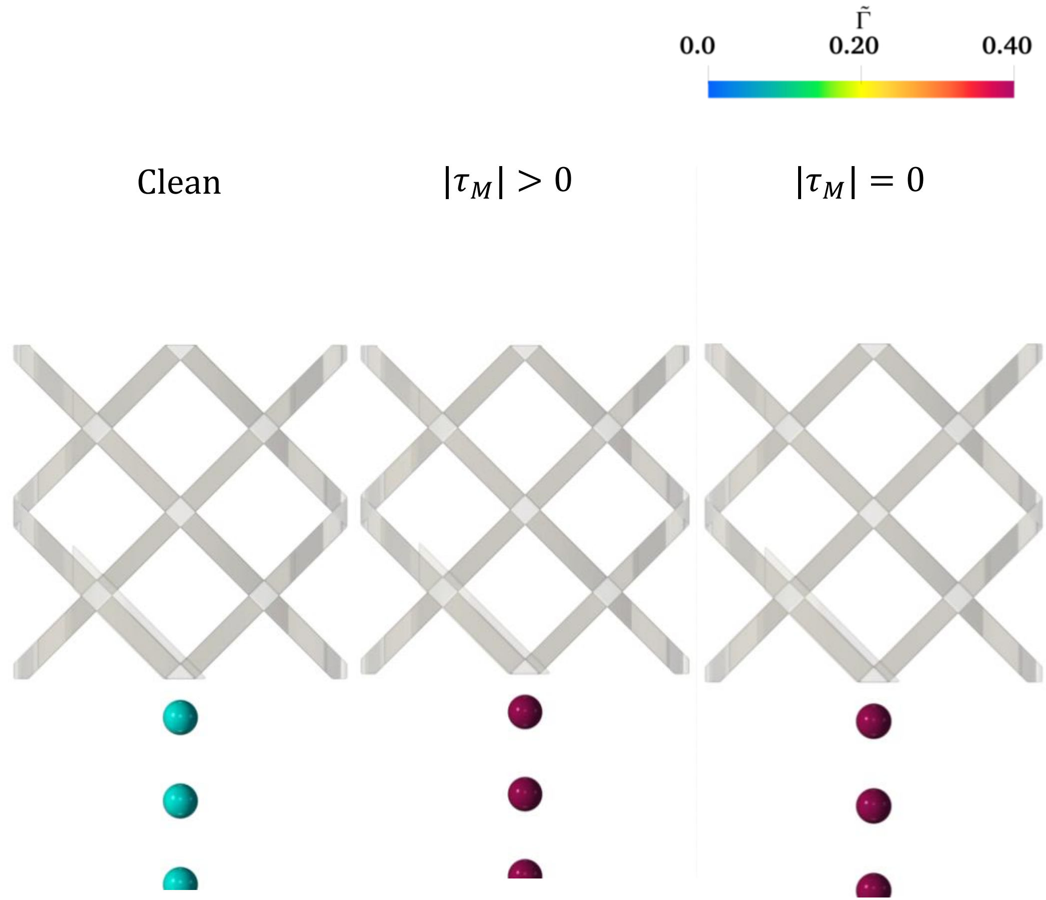
Juan Pablo Valdes [a,*], Lyes Kahouadji [a], Fuyue Liang [a], Seungwon Shin [b], Jalel Chergui [c], Damir Juric [c,d], Omar K. Matar [a]



Static Mixers

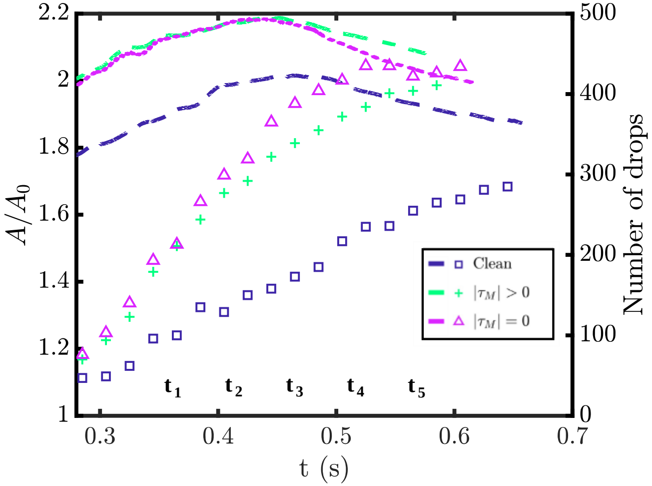
Dispersion Process: 1st Stage

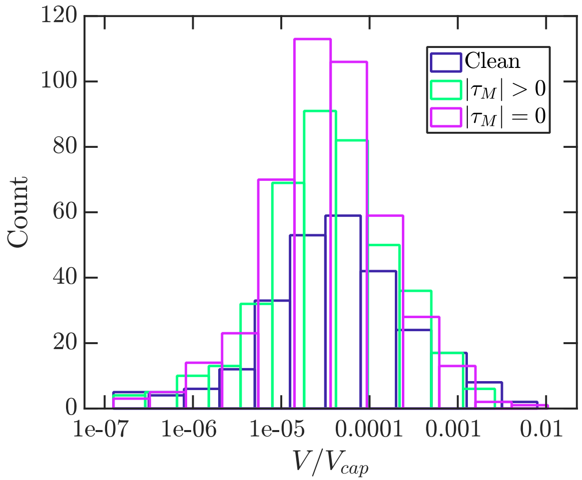


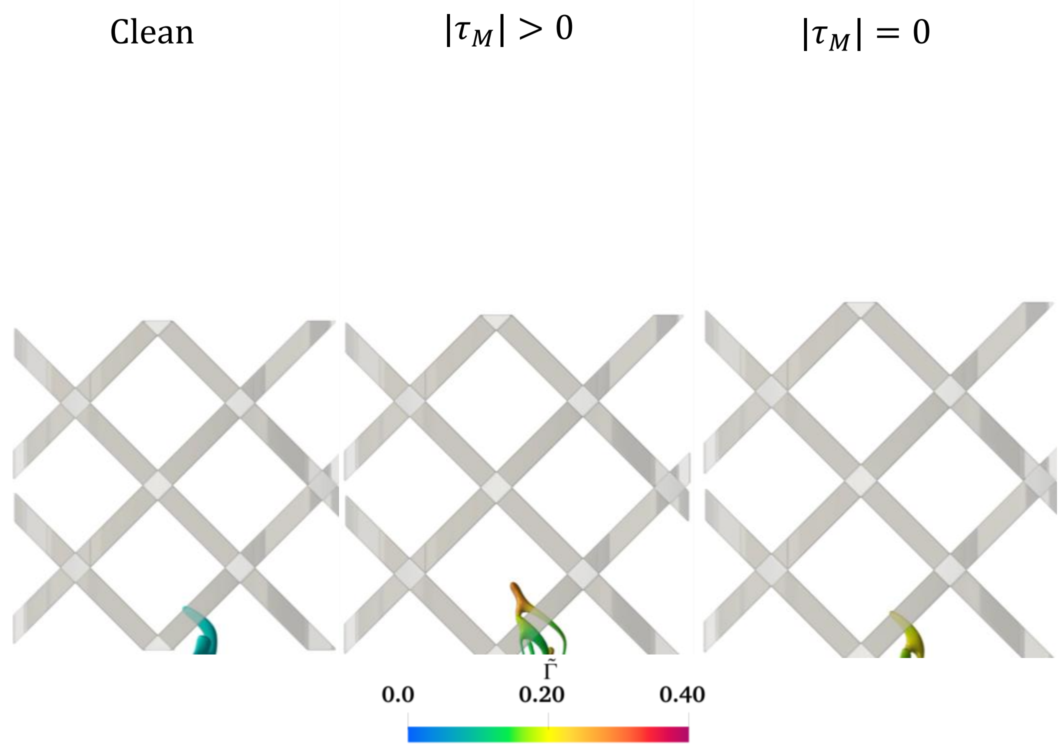


Static Mixers

Dispersion Process: 2nd Stage



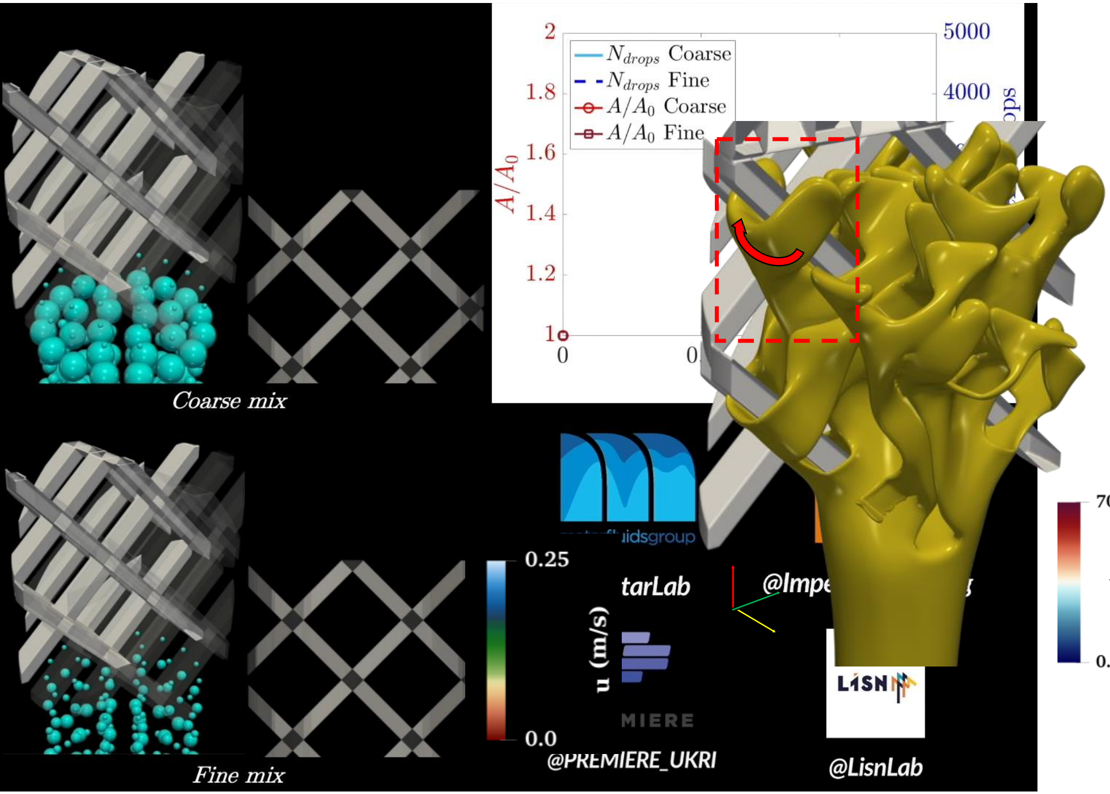


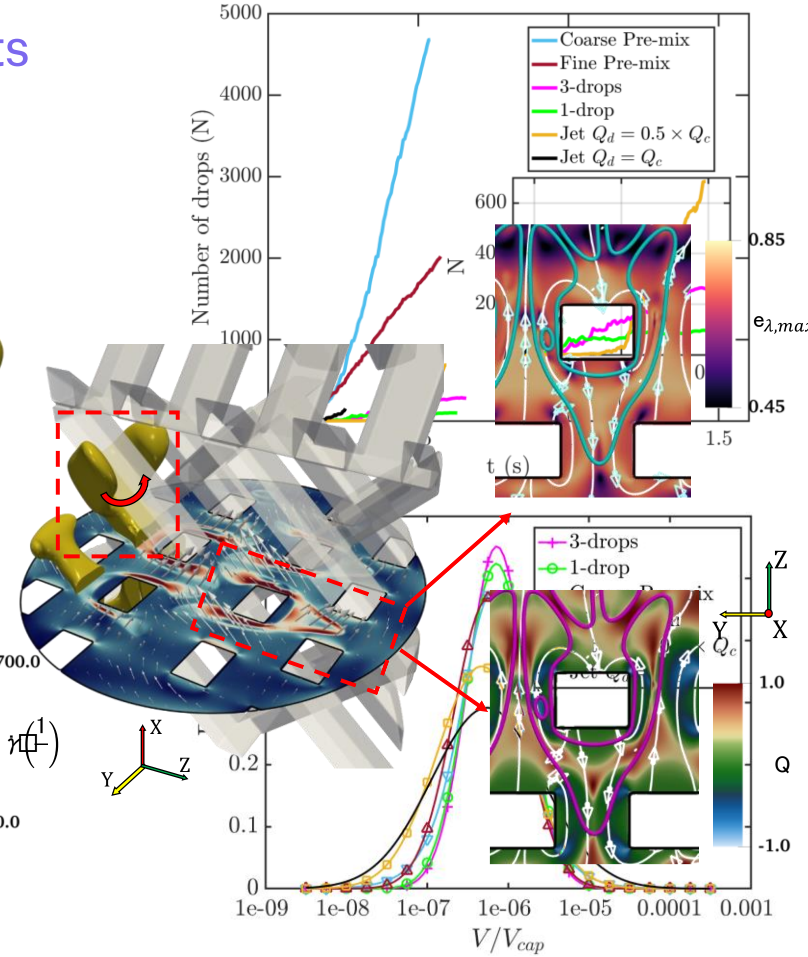


Imperial College London

Static Mixers

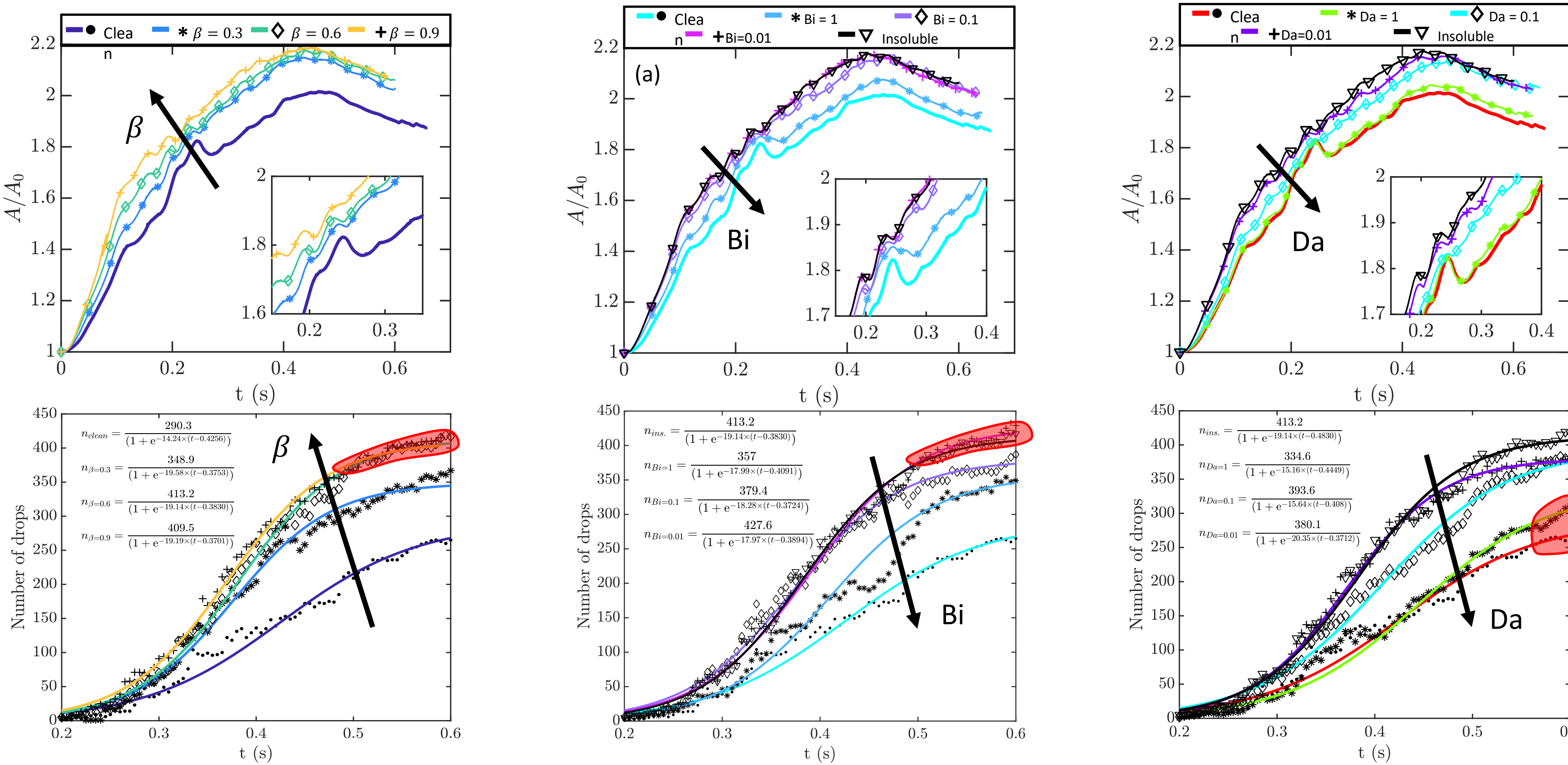
Complex Inlets



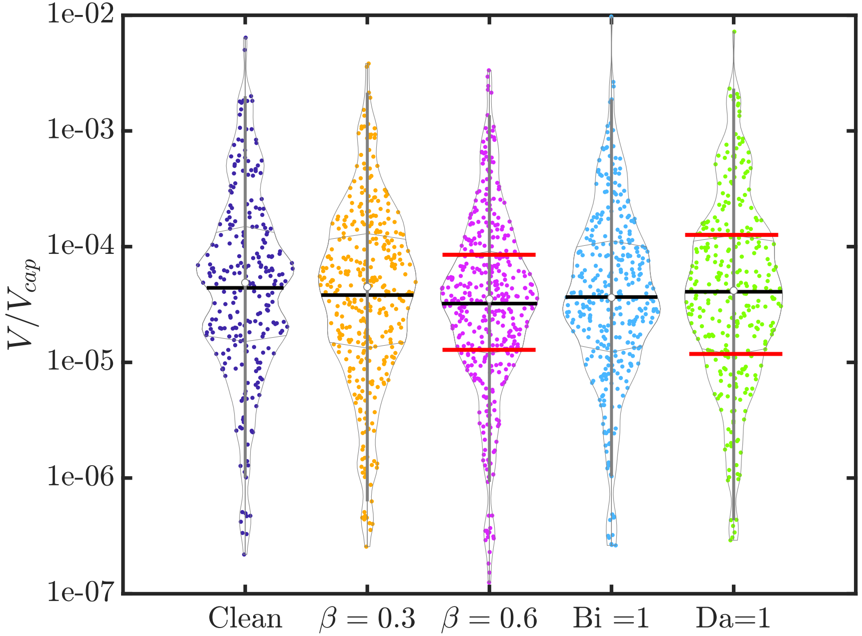


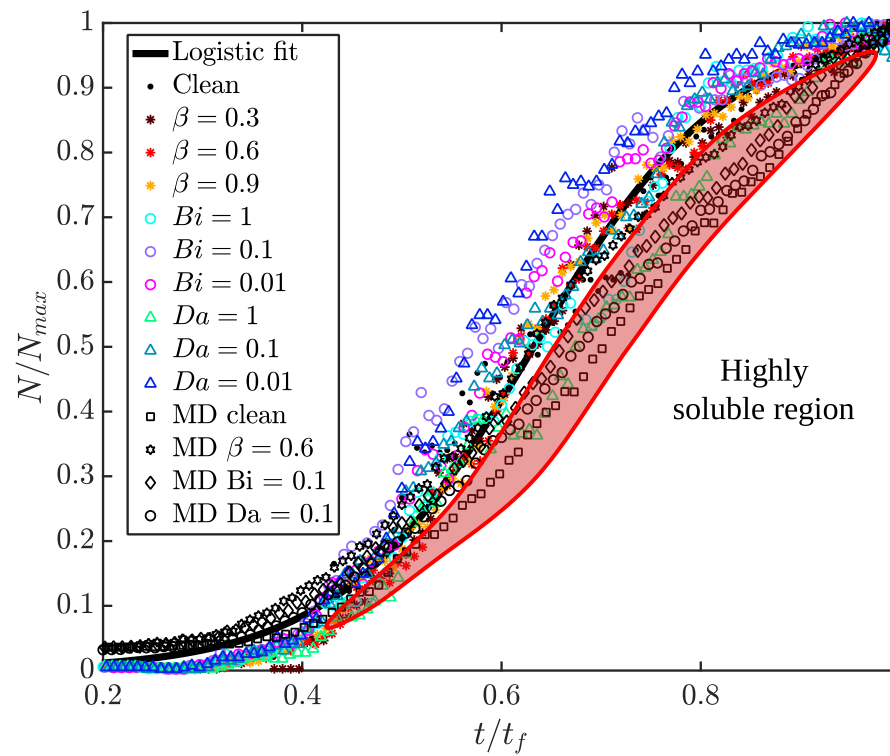
Static Mixers

Parametric Study



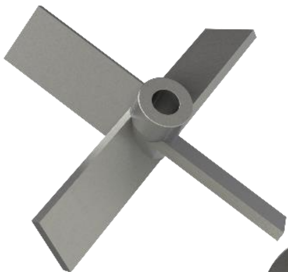
Static Mixers
Parametric Study





Stirred Vessels

Impeller Types

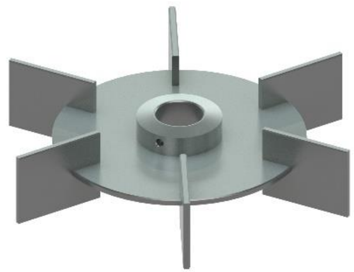


Axial Impeller

- Pitched blade turbine
- Hydrofoil
- Propeller

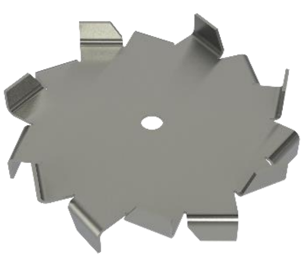
Radial Impeller

- Rushton turbine
- Smith RT



Others

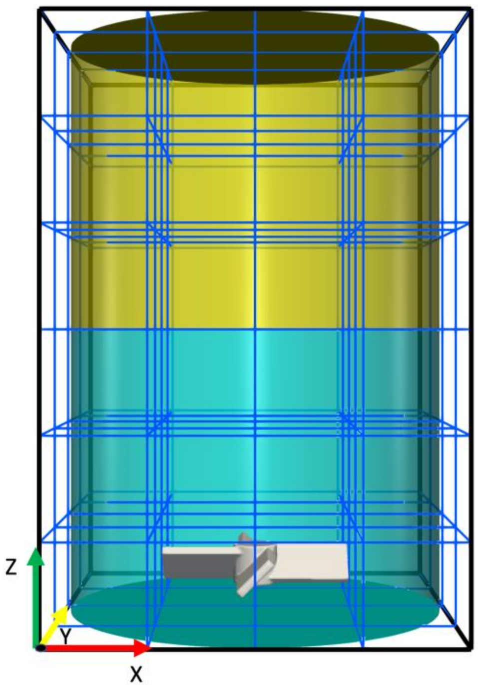
- Sawtooth Impeller
- Low level 'Kicker'
- folding impeller



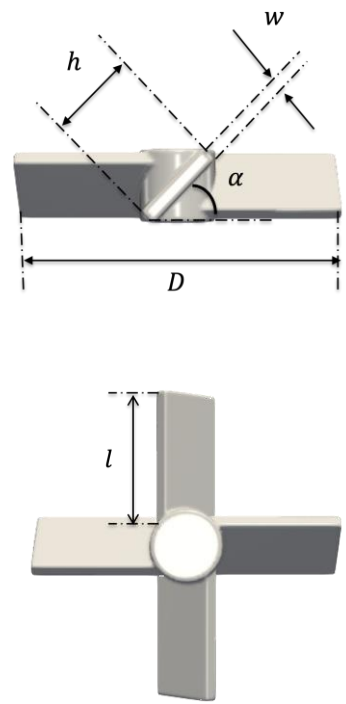
Close Clearance Impeller

- Anchor impeller
- Helical ribbon Impeller

Stirred Vessels
Simulation Setup



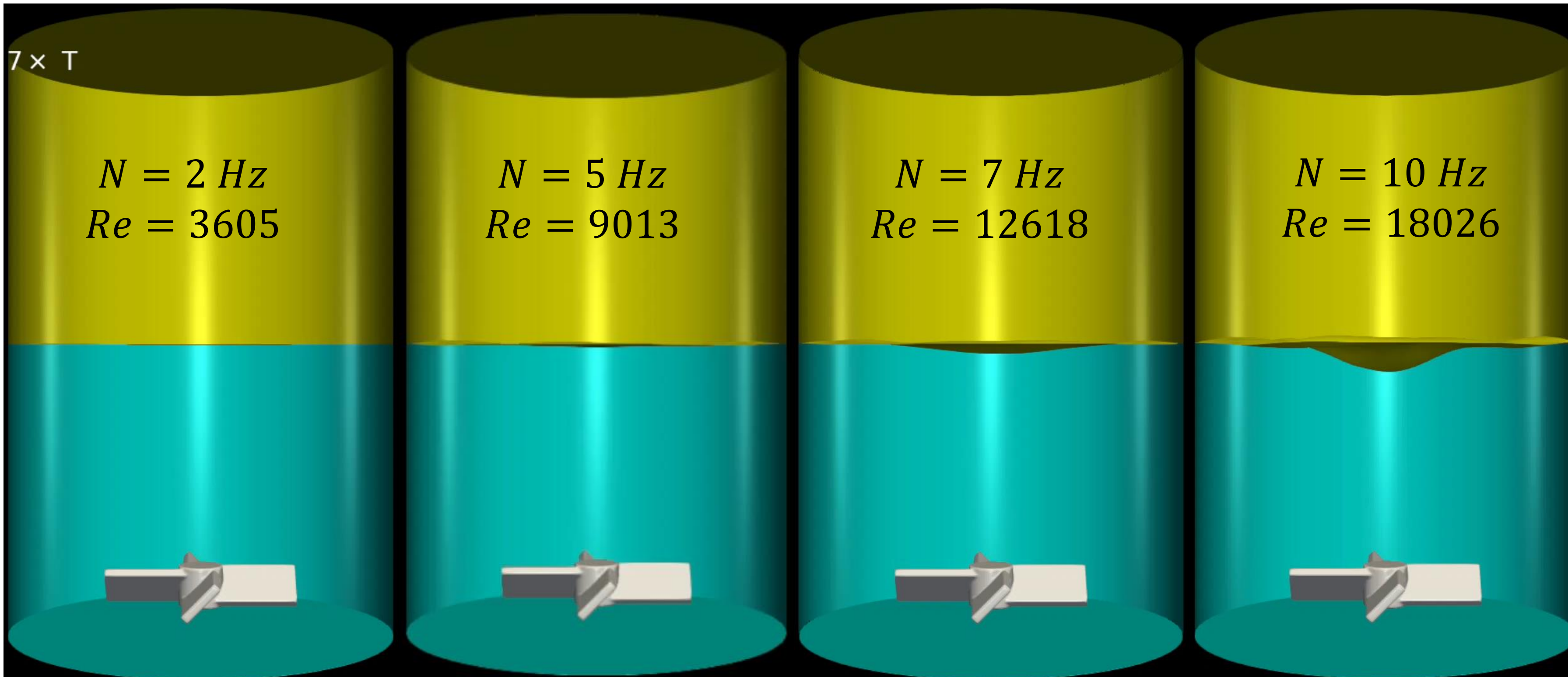
Tank dimensions [cm]	
Diameter T	8.5
Height, H	12.75
Computational resolution	
64x64x64 meshes in 4x4x6 subdomain	



Impeller Geometry [cm]	
diameter, D	4.25
height, h	1
thickness, w	0.2
length, l	2.5
clearance, C	1
inclined angle, α [°]	45
rotation speed, N [rps]	5
Physical properties	
surfactant-free interfacial tension, σ_s	0.035
oil viscosity, μ_o [Pa ·s]	5.4×10^{-3}
water viscosity, μ_w	1.0×10^{-3}
oil density, ρ_o [kg/m^3]	824
water density, ρ_w	998

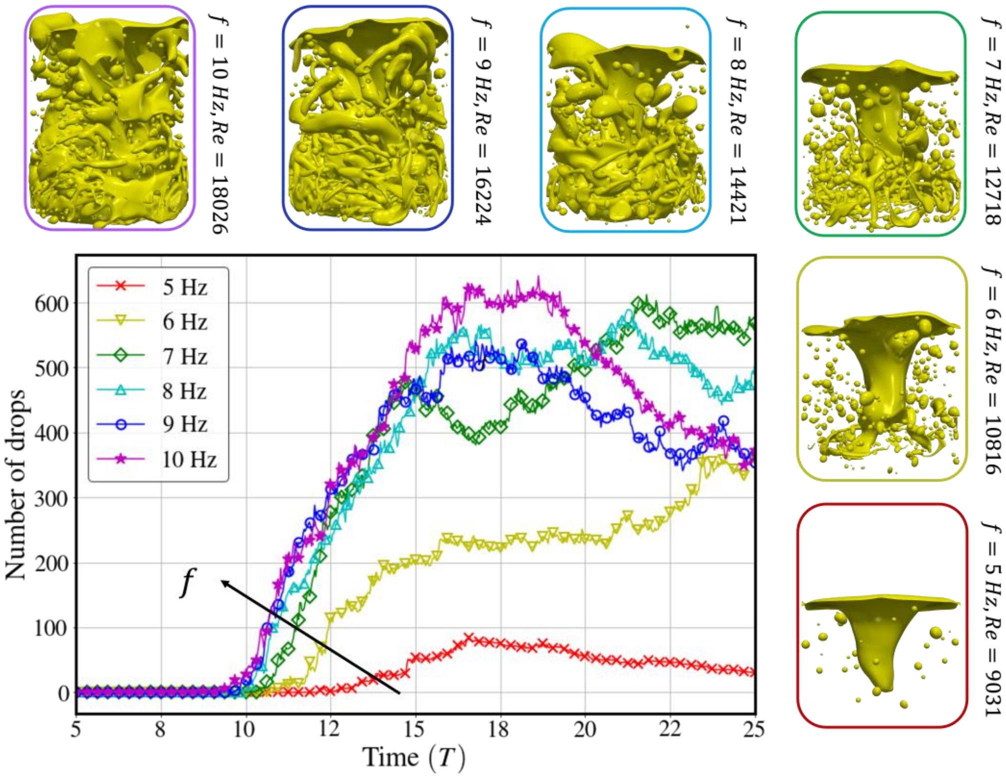
Stirred Vessels

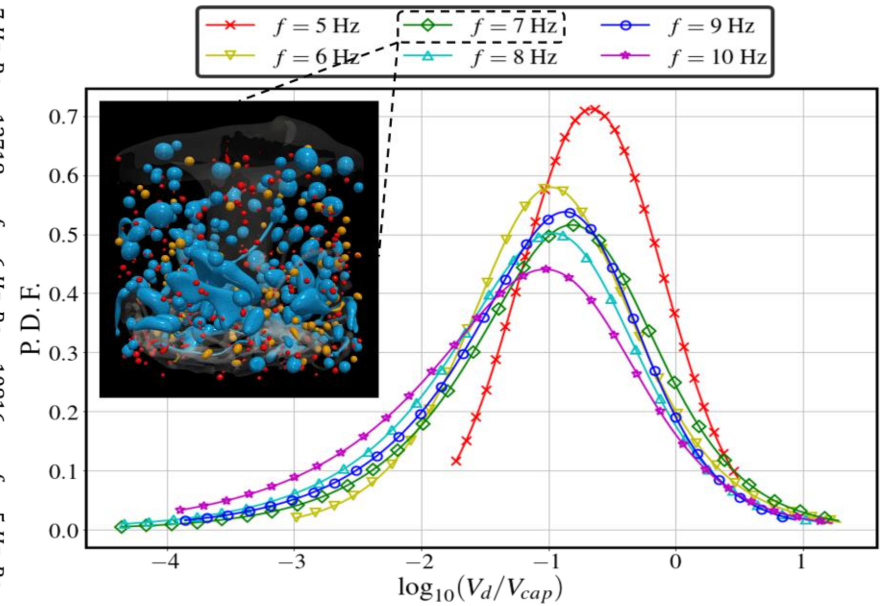
Effect of Impeller Speed



Stirred Vessels

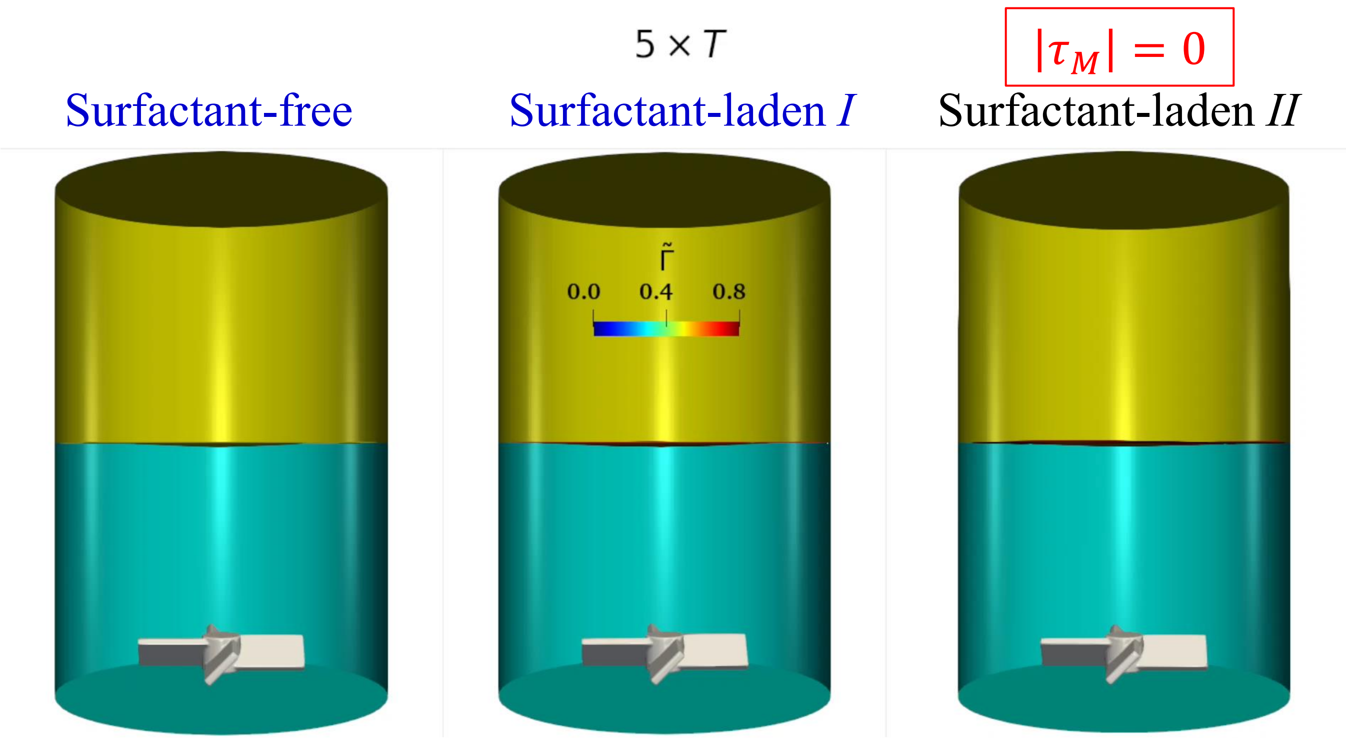
Drop Size Distributions





Stirred Vessels

Effect of Surfactant on Interfacial Dynamics



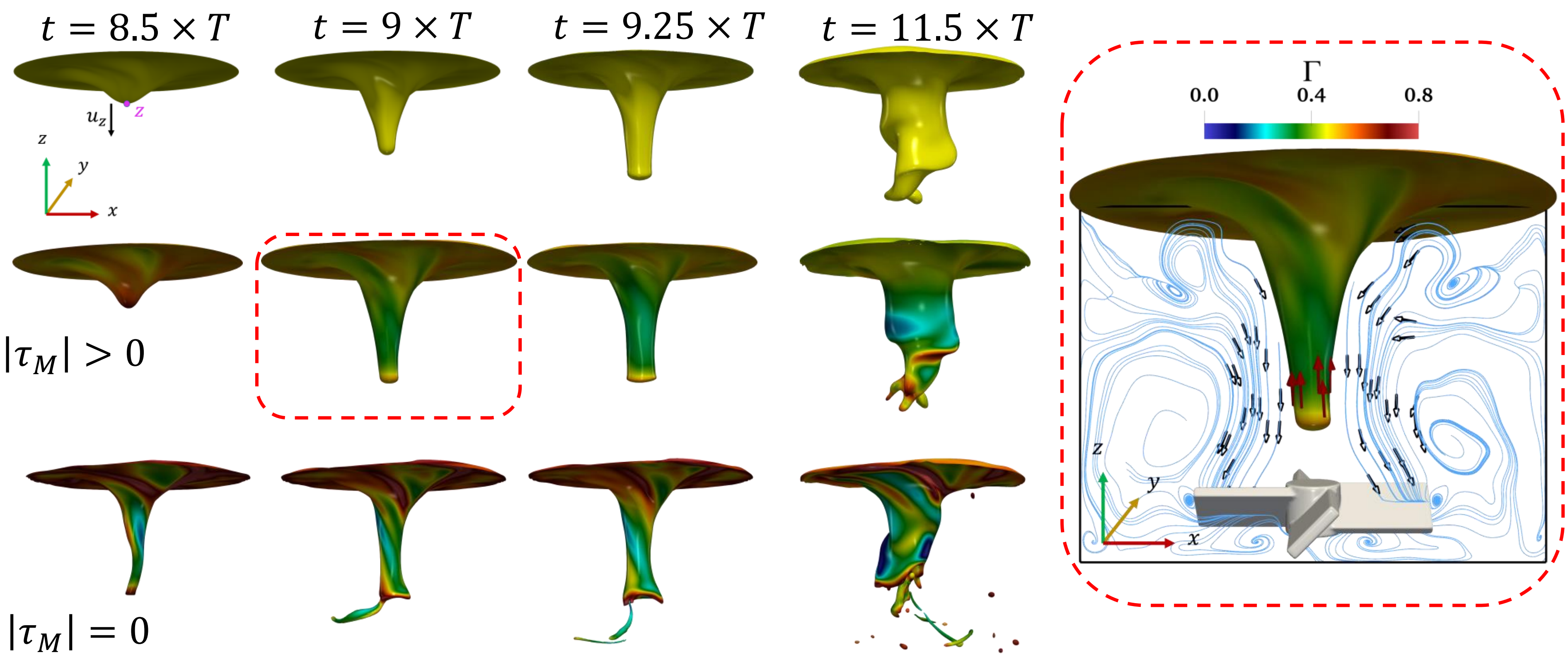
Step 1
Interface deformation

Step 2 & 3
Ligament and drop formation

Step 4
Cessation of interface-impeller contact

Stirred Vessels

Step 1: Interface Deformation

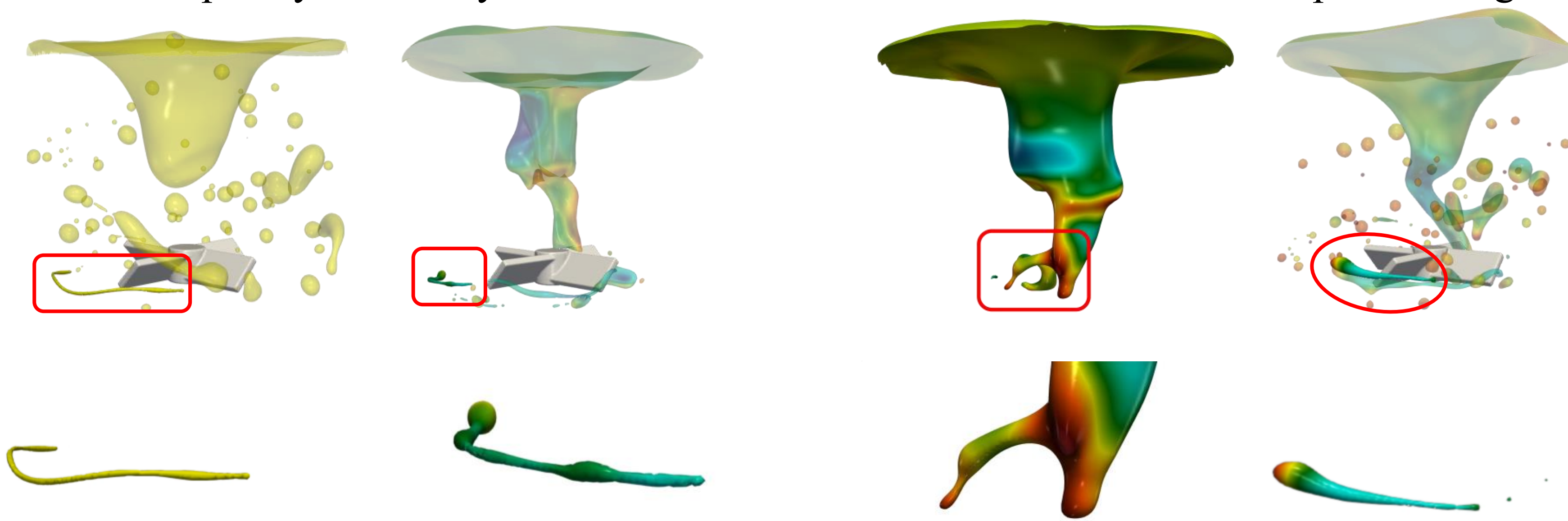


Stirred Vessels

Steps 2 & 3: Drop Dispersion

Mechanism 1:
Capillary instability

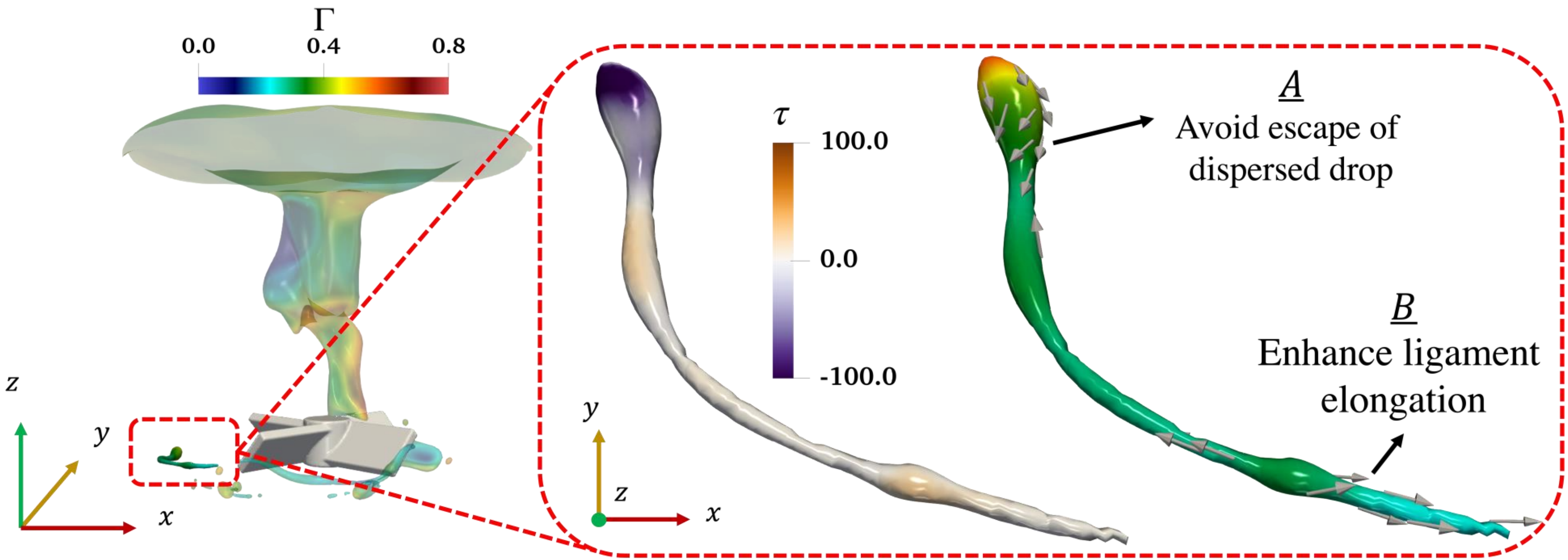
Mechanism 2:
Surfactant-enhanced tip streaming



Clean $t = 16.375 \times T$ | Surf. $t = 12.375 \times T$ | Surf. $t = 11.625 \times T$ | Surf. $t = 15.4 \times T$

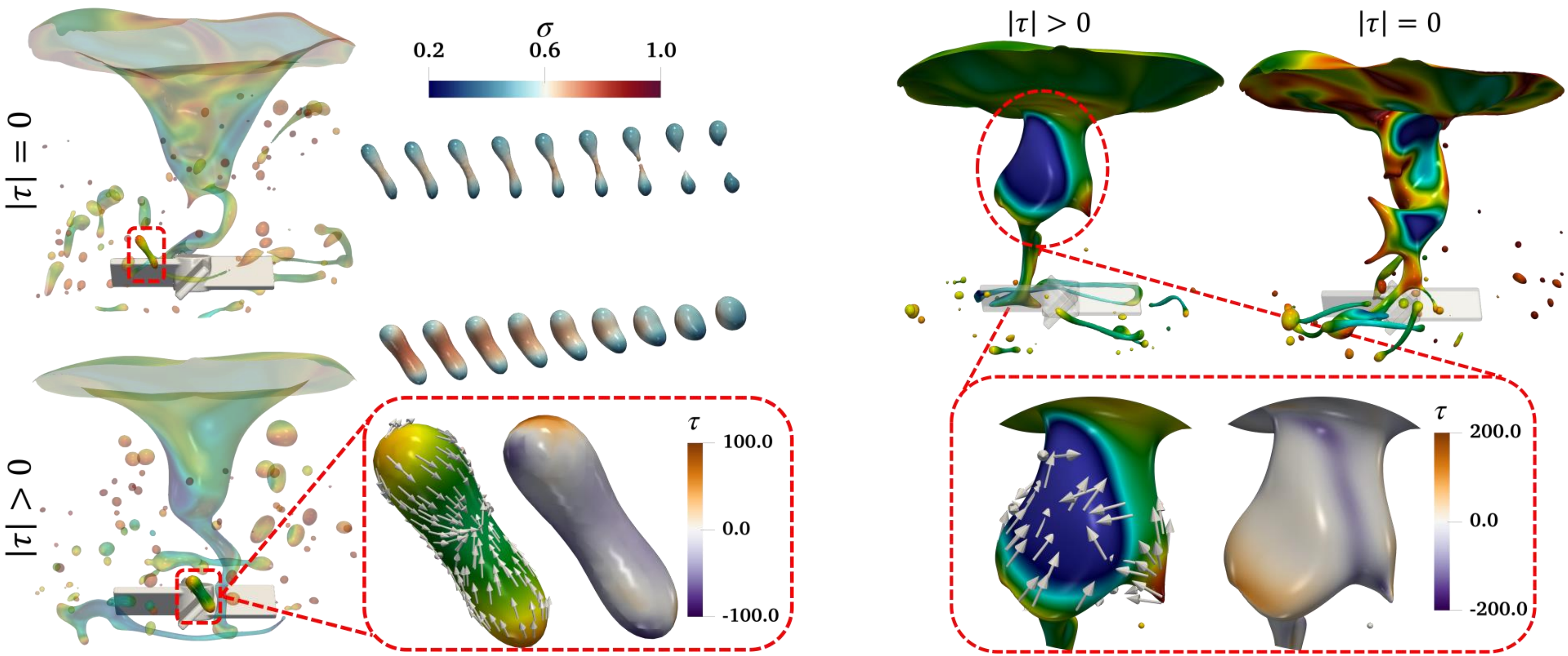
Stirred Vessels

Steps 2 & 3: Marangoni Effects



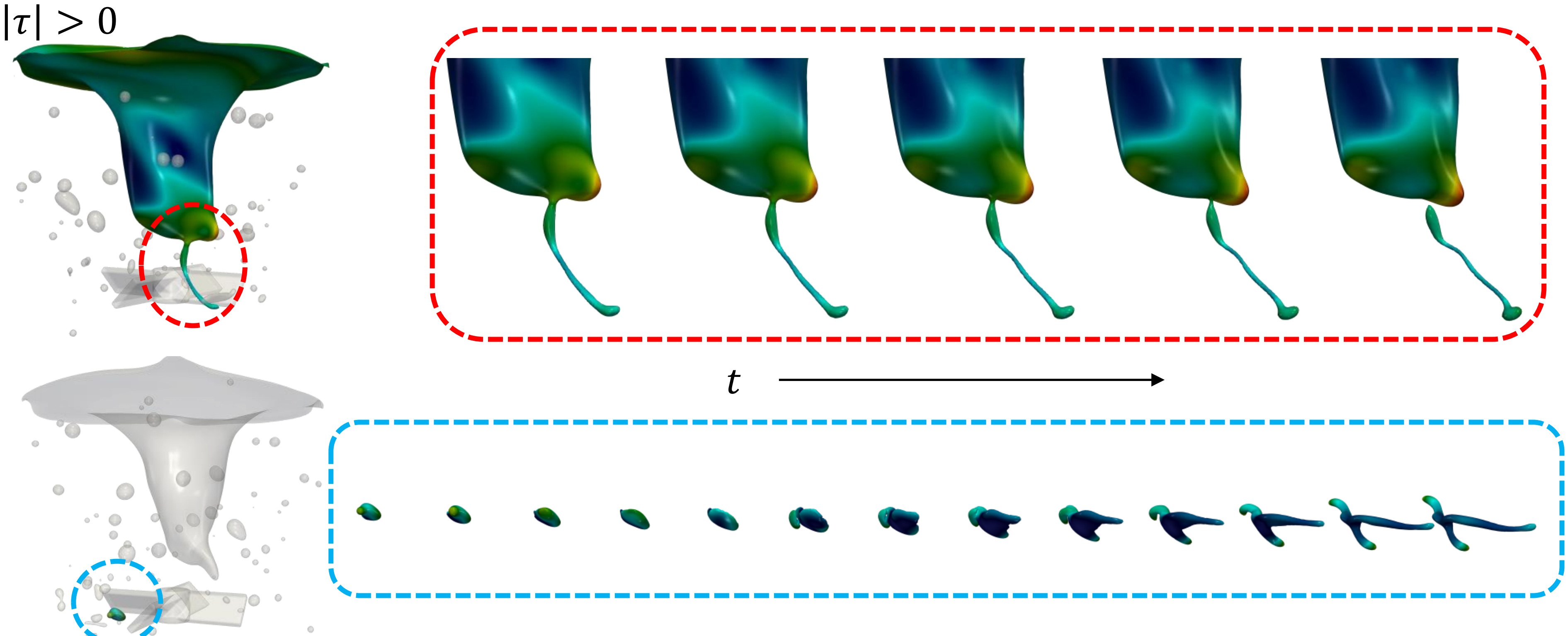
Stirred Vessels

Steps 2 & 3: Marangoni Effects

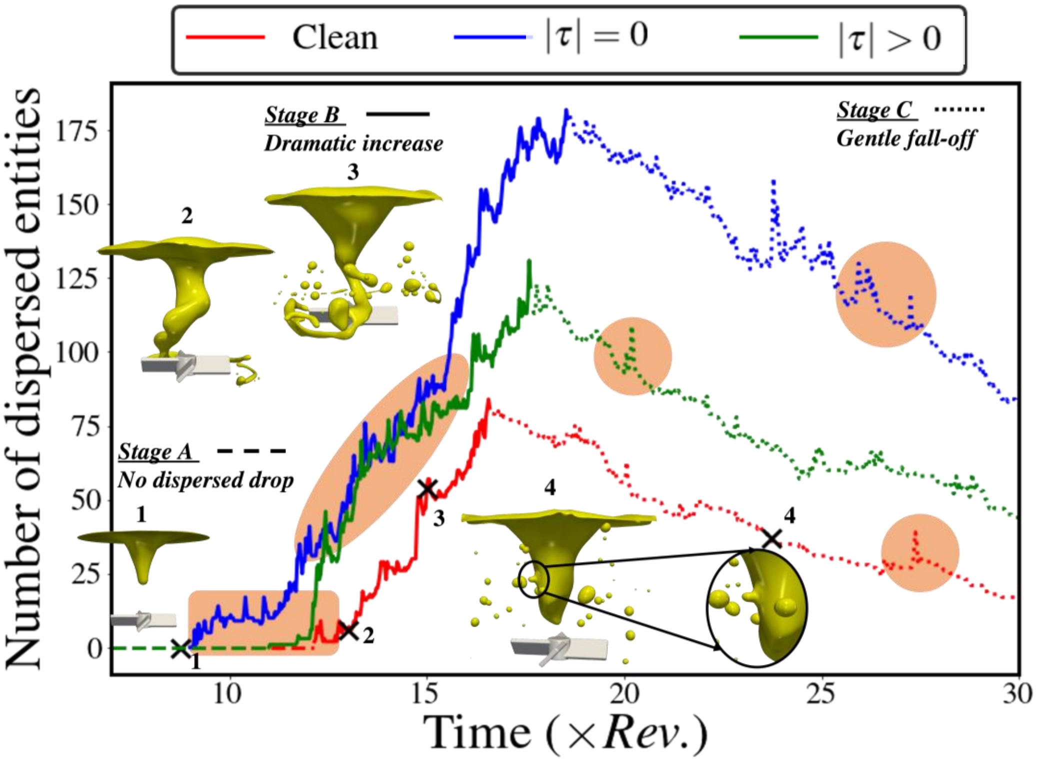


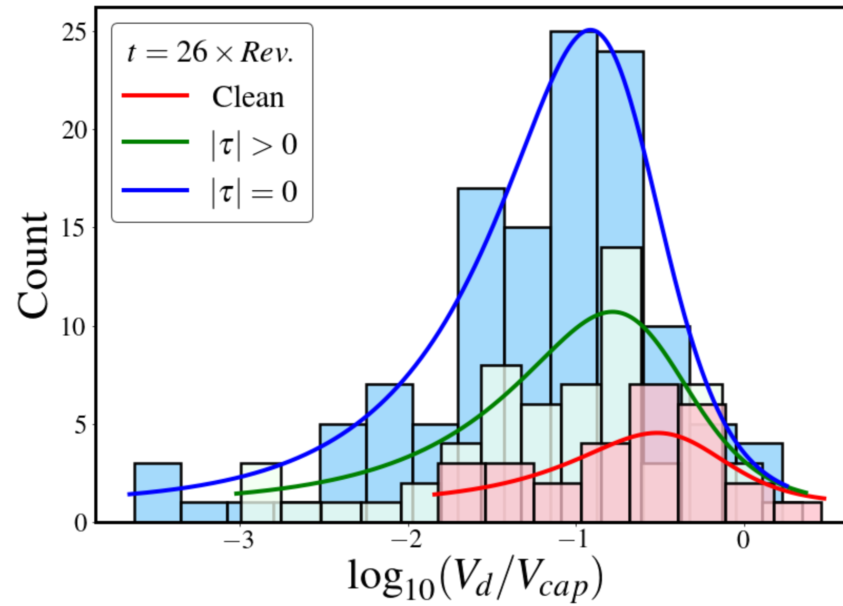
Stirred Vessels

Steps 4: Cessation of Interface-Impeller Contact



Stirred Vessels
Drop Number & Size Distribution





Acknowledgements













HONGIK UNIVERSITY

cnrs

UNIVERSITY OF CAMBRIDGE

UNIVERSITY OF OXFORD