Coalescence of Freely Suspended and Sessile Droplets

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Introduction

Key concepts:

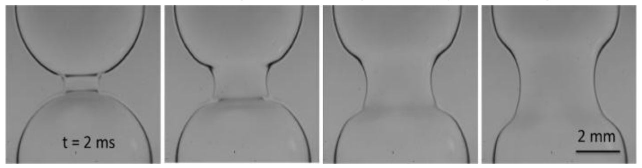
- ❑ Understand the coalescence dynamics of surfactant-laden droplets.
- ❑ Optimize the coalescence process and inform surfactant design for relevant applications.

Aim:

- ❑ Reveal the mass transport mechanism and the role of key parameters in the coalescence of freely suspended and sessile surfactant-laden droplets.

Applications:

- ❑ Microfluidics, Inkjet printing, Spray cooling



Experimental image showing droplet coalescence (aqueous solution SLES) [1]

Model and Methodology

Model:

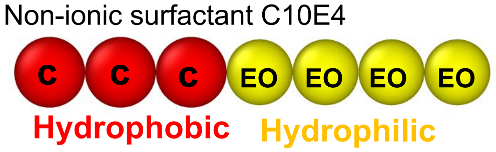
- ❑ SAFT(Statistical Associating Fluid Theory) coarse-grained force-field based on the Mie potential [2]

Method:

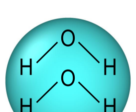
- ❑ Molecular dynamics simulation
- ❑ NVT ensemble

Materials:

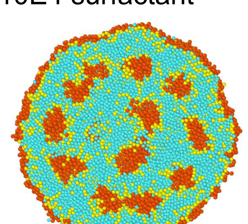
- ❑ Water
- ❑ Non-ionic surfactant C10E4



SAFT representation of C10E4 surfactant



Water bead in SAFT force field



Morphology of a surfactant-laden droplet at equilibrium (C = 35.5 wt [%])

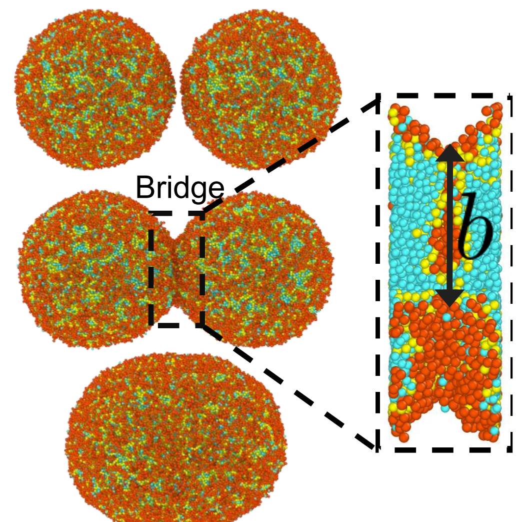
Model and Methodology

Name	Particle type (SAFT)
Alkane -CH2-CH2-CH2-	C
Oxyethylene -CH2-O-CH2-	EO

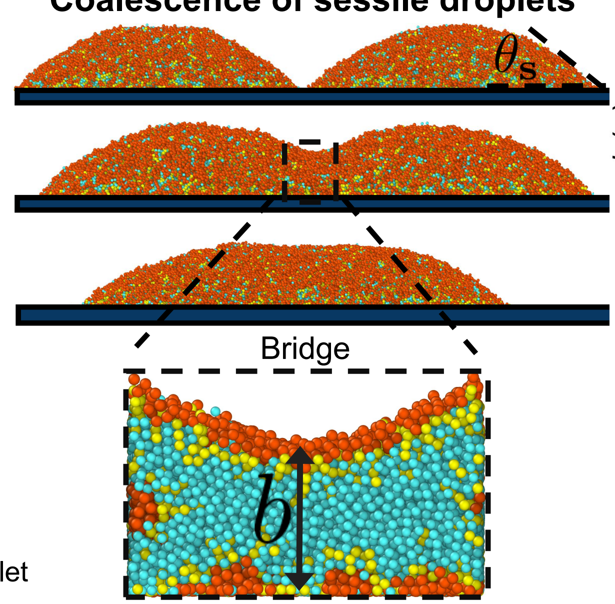
C10E4 beads definition in SAFT force field [2]

Results

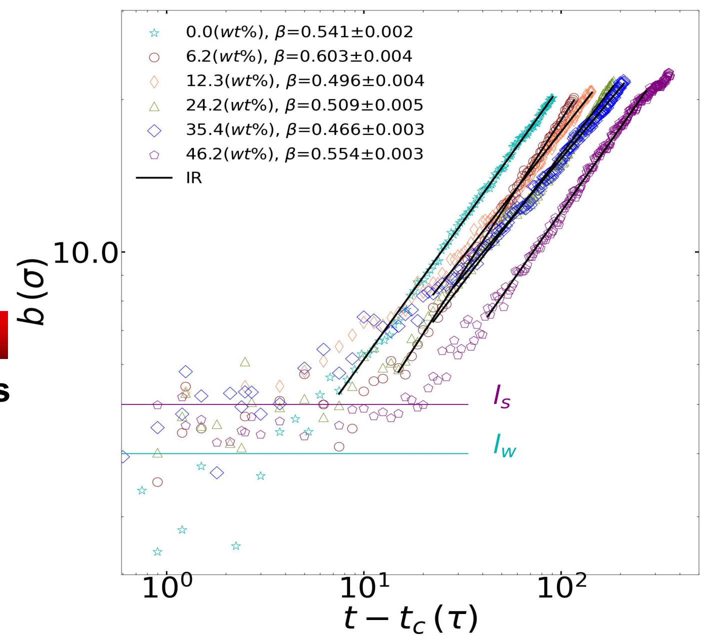
Coalescence of suspended droplets



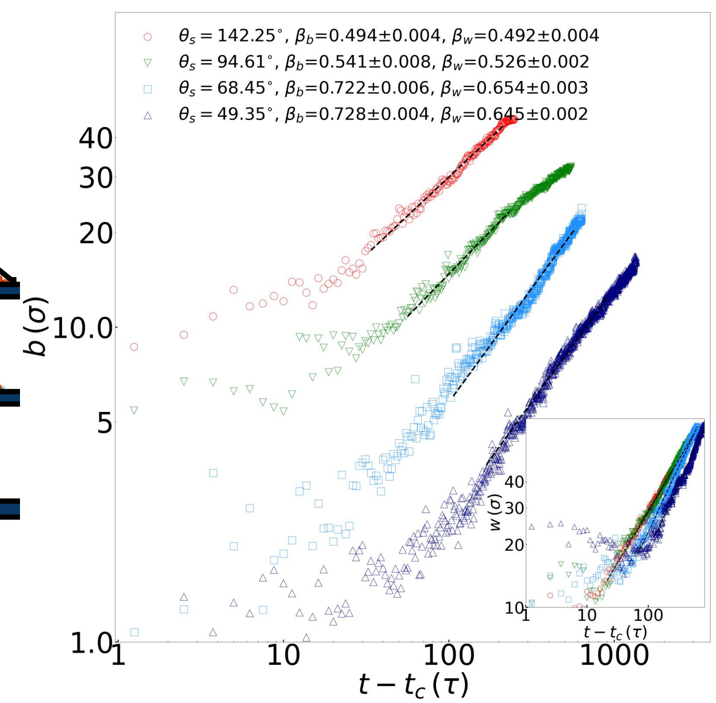
Coalescence of sessile droplets



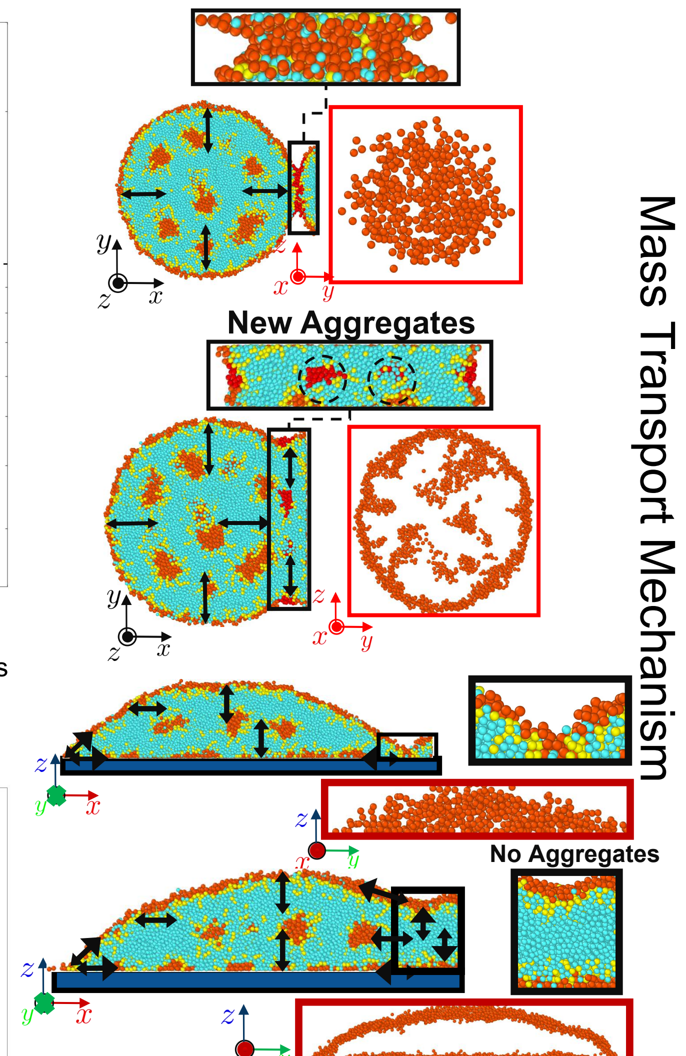
Results



Bridge growth dynamics [3,4] of suspended droplets
Two regimes:Thermal and Inertial (power law 0.5)



Bridge growth dynamics of Sessile droplets
Two regimes:Thermal and Inertial: (power law 0.5 for $\theta_s \geq 90^\circ$ and power law 0.7 for $\theta_s < 90^\circ$)



Conclusion

- ❑ Examination of Mass Transport Mechanism and Bridge Growth Dynamics during the Coalescence of Freely Suspended and Sessile Surfactant-Laden Droplets.
- ❑ Identification of Two Bridge Growth Regimes: Thermal Regime (TR) and Inertial Regime (IR).
- ❑ Observation of New Surfactant Aggregates Forming Inside the Bridge Bulk in Freely Suspended Droplets, Absent in Sessile Droplets.

References:

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[2] Avendaño, Carlos, Thomas Lafitte, Claire S. Adjiman, Amparo Galindo, Erich A. Müller, and George Jackson. J.Phys. Chem. B 2013, 117, 9, 2717–27333

[3] **Soheil Arbabi, Piotr Deuar, Mateusz Denys, Rachid Bennacer, Zhizhao Che, Panagiotis E. Theodorakis**; Coalescence of surfactant-laden droplets. Phys. Fluids 35 063329 (2023)

[4] **Soheil Arbabi, Piotr Deuar, Mateusz Denys, Rachid Bennacer, Zhizhao Che, and Panagiotis E. Theodorakis**. "Molecular dynamics simulation of the coalescence of surfactant-laden droplets." Soft Matter 19, 8070-8080 (2023)

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