Coalescence of surfactant-laden droplets

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Introduction

Key concepts:

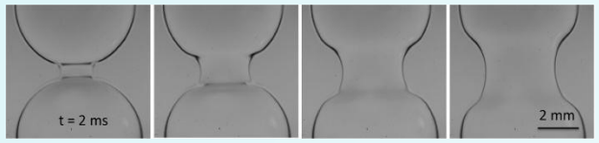
- Understand the coalescence dynamics of surfactant-laden droplets
- Optimize the coalescence process and inform surfactant design for relevant applications

Aim:

- Reveal the mass transport mechanism and the role of key parameters in coalescence process

Applications:

- Microfluidics, Inject printing, Spray cooling



Experimental image of droplets 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 and NPT ensembles)

Materials:

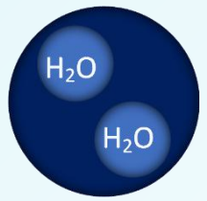
- Water
- Non-ionic surfactant C10E8

SAFT representation of C10E8 surfactant

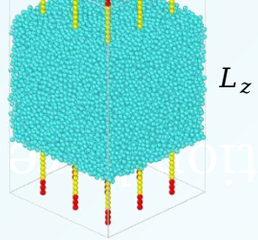
Model and Methodology

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

C10E8 beads definition in SAFT force field [2]

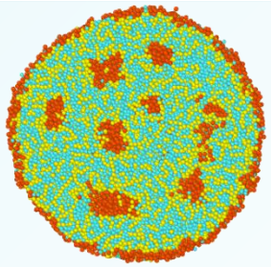


Water bead in SAFT force field



Water and surfactant slab geometry for surface tension

Results

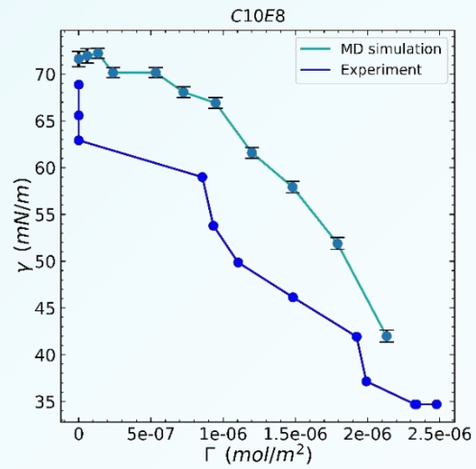


Morphology of a surfactant-laden droplet at at equilibrium (C=50%)

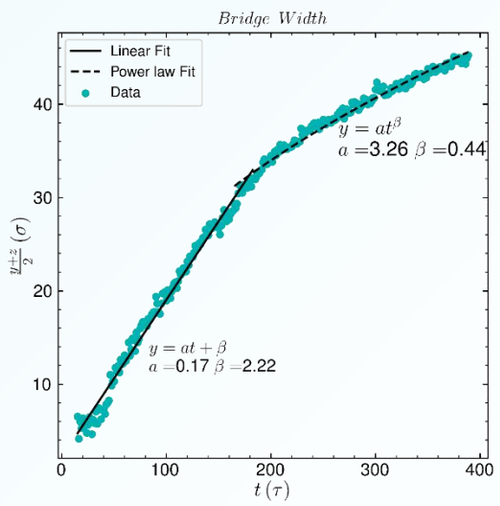
Evaluation of water surface tension (Mechanical way), based on the relation:

$$\gamma = \frac{L_z}{2}\left[P_{zz} - \left(\frac{P_{xx}+P_{yy}}{2}\right)\right]$$

Results



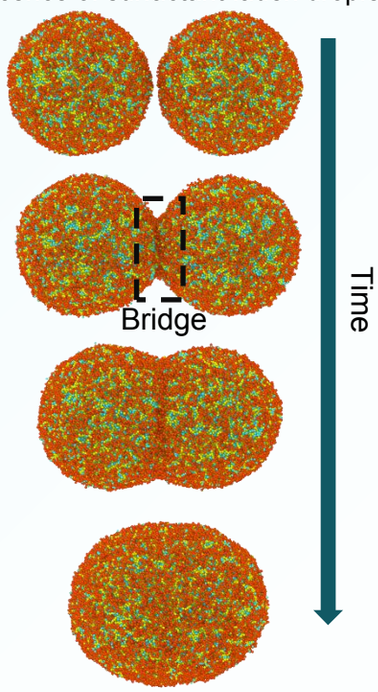
Surface tension of Water-C10E8 mixture (25 °C): Pure water surface Tension ~72 mN/m



Bridge between two droplets grows with two different regimes: Inertial (linear) and Viscous (power law 0.5)

Results

Coalescence of surfactant-laden droplets



Conclusion

- The SAFT coarse grained force-field indicates a close match with experimental results in terms of surface tension and water-surfactant interaction.
- We have presented examples of surfactant-laden droplet coalescence and bridge growth dynamics.

References:

1. E. Nowak, N.M. Kovalchuk, Z. Che, M.J.H. Simmons. Colloids Surf. A. 505:124-131 (2016)
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

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