# Coalescence of Surfactant-laden Droplets

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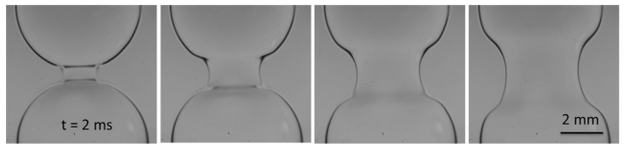
## Introduction

- **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

- **Applications:**
- Microfluidics, inkjet printing, spray cooling, bio-process



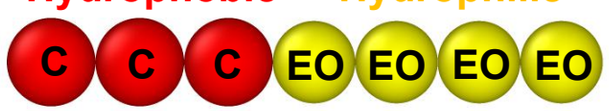

Experimental image of droplets coalescence (aqueous solution SLES)
Figure from [1]

## Model and Methodology

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

**Method:**
- Molecular dynamics simulation (NVT)

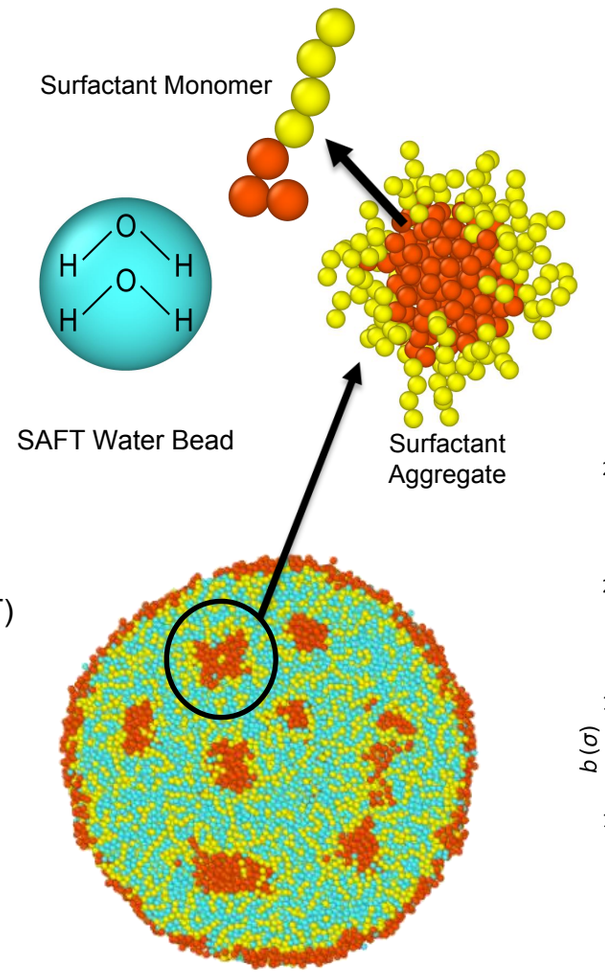
**Materials:**
- Water
- Non-ionic surfactant C10E4




## Model and Methodology

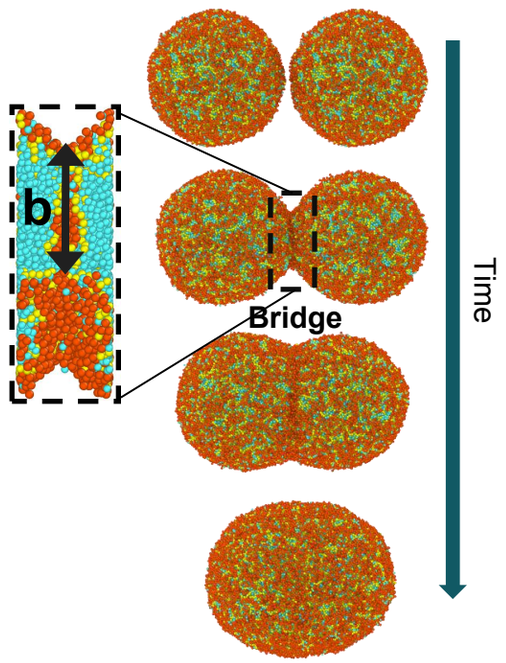
| Name | Particle type (SAFT) |
|---|---|
| Alkane –CH2–CH2–CH2– | C |
| Oxyethylene –CH2–O–CH2– | EO |
| Water | W |

C10E4 beads definition in SAFT force field [2]

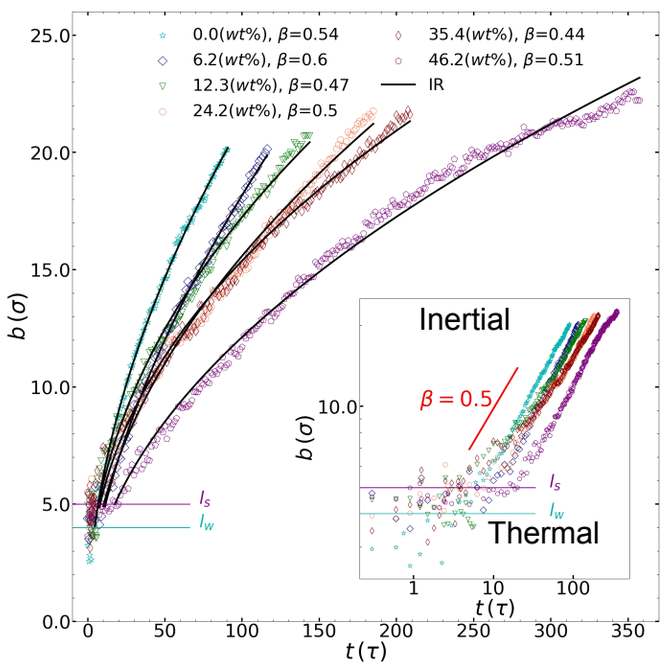



## Results

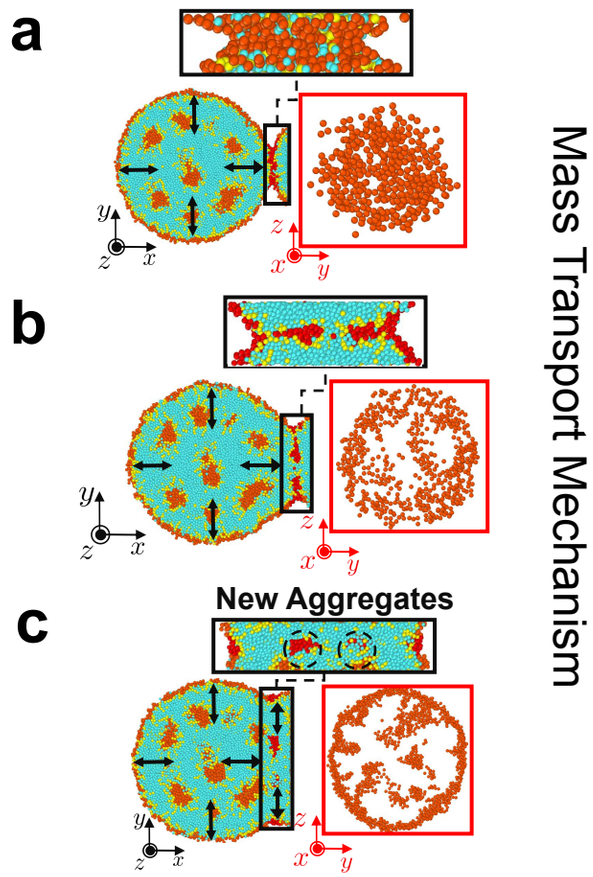
**Stages of Coalescence**




**Bridge growth dynamics**




## Results




## Conclusions

- Two different regimes of bridge growth dynamics are identified: Thermal and Inertial.
- Mass transport Mechanism:

**a)** Pinching with contribution of surfactant hydrophobic beads.

**b)** Movement of surfactant molecules from bridge bulk towards the bridge surface.

**c)** Creation of new aggregates inside the bridge bulk and no significant mass transport between bulk and surface after the bridge has fully developed.

**References:**
1. E. Nowak, N.M. Kovalchuk, Z. Che, M.J.H. Simmons. Colloids Surf. A. 505:124-131 (2016)
2. T.Lafitte, A.Apostolakou, C.Avendaño,A.Galindo,C.S. Adjiman, E.A. Müller and G.Jackson J. Chem. Phys. 139, 154504 (2013)

**Acknowledgment:**
This research has been supported by the National Science Centre, Poland, under grant No. 2019/34/E/ST3/00232. This research was supported in part by PLGrid Infrastructure.