Thermal Fluctuation break-up of Surfactant-Laden Liquid Threads

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Introduction

Key Concept: The formation of droplets from a liquid jet is influenced by surfactants and thermal fluctuations.
Aim: Understand the mechanism of breakup that leads to the formation of droplets and satellite droplets at the molecular scale.
Applications: Inkjet printing, microfluidic devices

Model and Methodology

Method: Many-body dissipative particle dynamics simulations of a cylindrical liquid geometry were realized with the goal to reproduce the Rayleigh-Plateau instability on systems with different surfactant concentrations. MPDP was chosen for this problem due to its lower computational cost when compared to traditional MD. It is a particle based coarse grained method with soft interactions and a Langevin type thermostat.

Analysis: Many simulations were realized to obtain statistical information of various system properties. We track the distribution of surfactant molecules to elucidate its transport mechanism as the pinch off occurs and we compare the minimum radius scaling with theoretically proposed breakup regimes.

Results

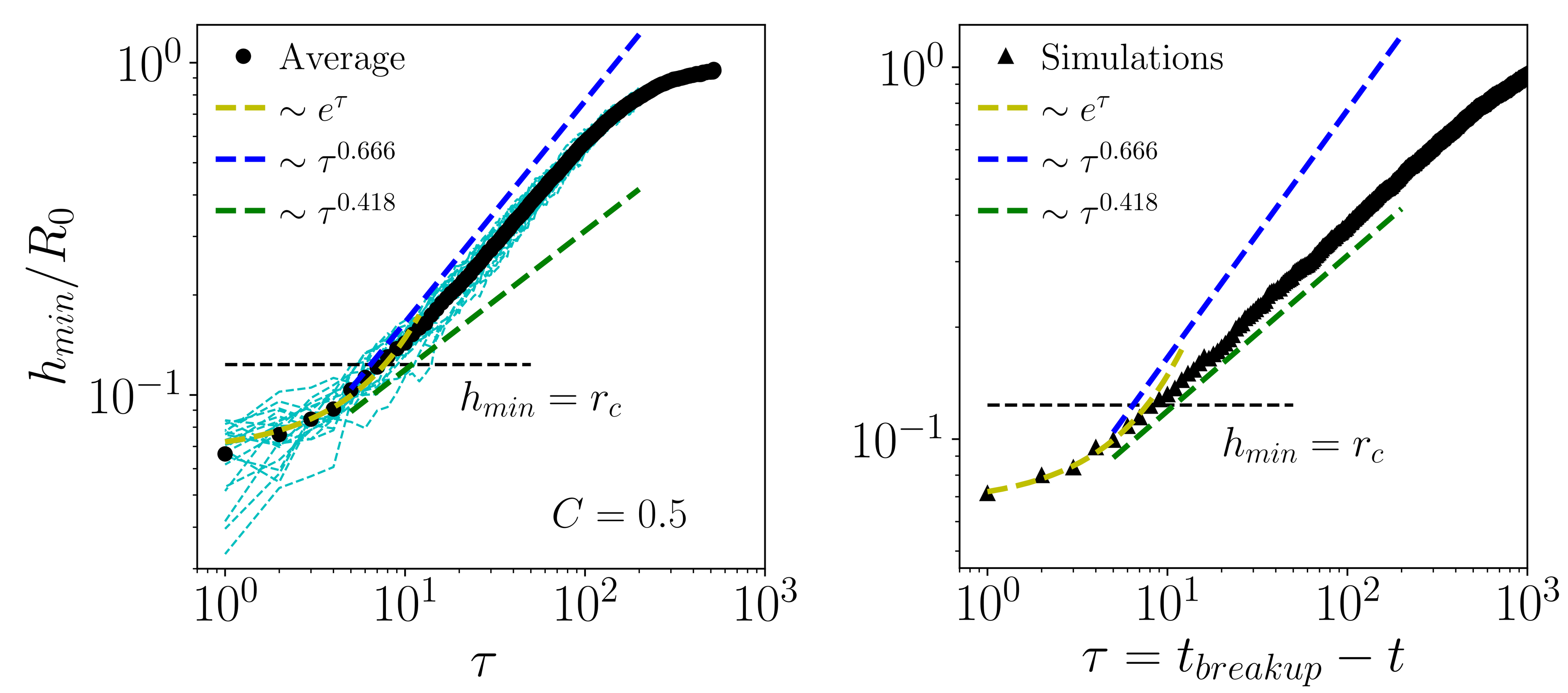

Figure: Thinning dynamics of the pinching point for threads below and above CMC (left and right respectively). Dashed lines are only references to compare the results.

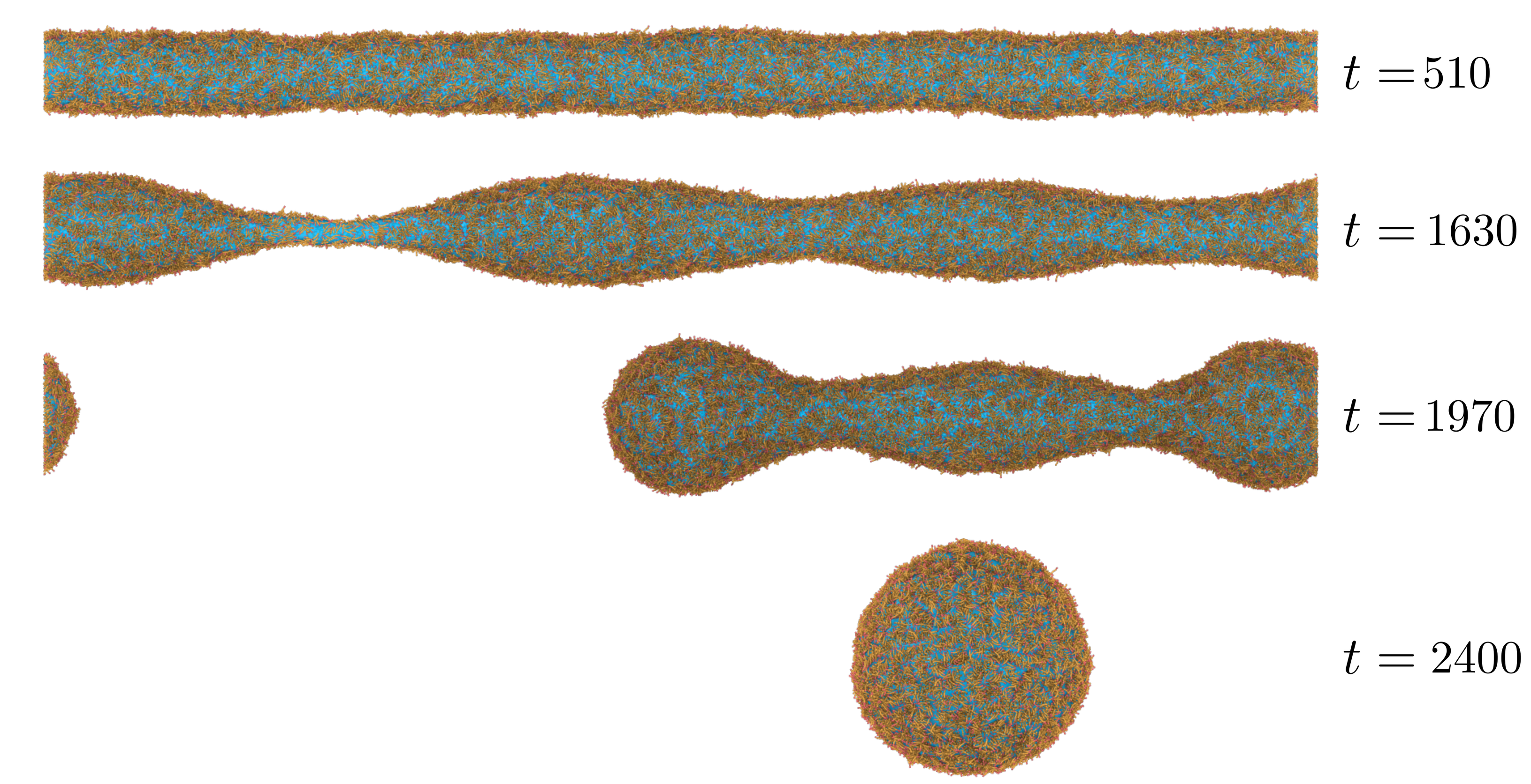

Figure: Time evolution of the breakup of a liquid thread with surfactants. Time is in MDPD units.

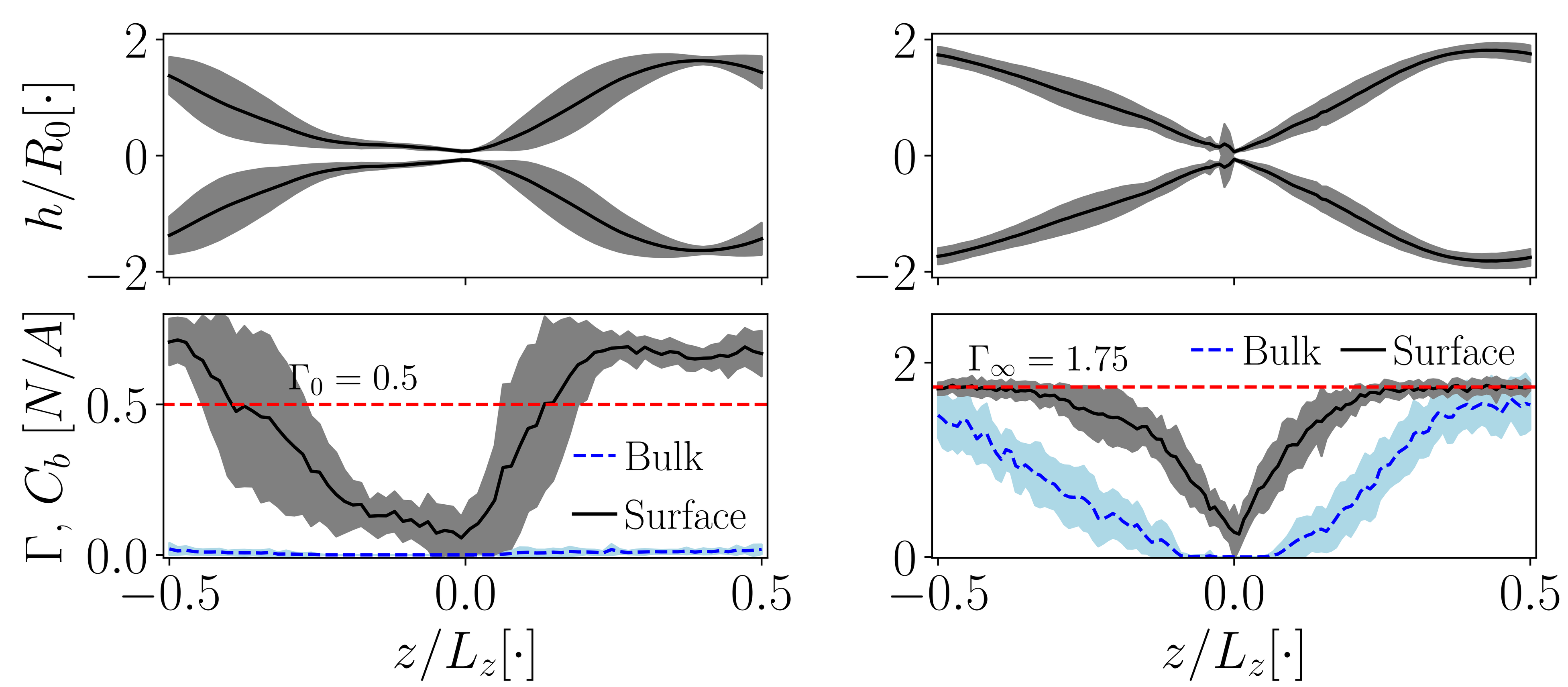

Figure: Breakup profiles below and above CMC (left and right respectively) and surfactant distribution along the z axis. Lines represent the average from 20 simulations and shaded area is one standard deviation.

Conclusions

- Transition between inertial breakup regime at low surfactant concentrations to a Thermal fluctuation regime at a higher concentration;
- Possible exponential regime found when the thread radius reaches the MDPD interaction cutoff;
- Surfactant molecules are advected away from the pinching point towards the main droplet until the surface excess concentration reaches a saturation level. After this point, they start to move into the bulk phase.

1) L. H. Carnevale, P. Deuar, Z. Che, P. E. Theodorakis. Physics of Fluids 2023; 35 (7): 074108. https://doi.org/10.1063/5.0157752

2) L. H. Carnevale, P. Deuar, Z. Che, P. E. Theodorakis. (2024 – Under Review)

Acknowledgment:
Supported by the NCN, Poland, grant No. 2019/34/E/ST3/00232 and by PLGrid Infrastructure, grant No. PLG/2022/015747 .