

Abstract

Formation of Pure and Surfactant-laden Droplets with Many-body Dissipative Particle Dynamics

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This thesis employs many-body dissipative particle dynamics (MDPD) to investigate the molecular mechanisms underlying the breakup of pure and surfactant-laden liquid threads. MDPD is a particle-based mesoscale simulation technique that captures thermal fluctuations and soft-core interactions, bridging molecular and macroscopic scales. By simulating the Rayleigh–Plateau instability, MDPD provides critical insights into how molecular forces and thermal fluctuations influence droplet formation at nanoscales.

Surfactants, which adsorb at liquid interfaces and reduce surface tension, play a crucial role in altering the breakup dynamics of liquid threads. Their presence introduces additional complexity by driving Marangoni flows due to surface tension gradients. MDPD simulations demonstrate how surfactant concentration affects droplet size, distribution, and the formation of undesirable satellite droplets, offering strategies to mitigate these effects.

This study focuses on the interplay between molecular interactions and fluid instability during liquid thread breakup, highlighting how molecular-level mechanisms contribute to different breakup regimes. The findings advance the understanding of the Rayleigh–Plateau instability and provide practical insights for optimizing droplet formation in applications requiring precise control over fluid behavior.

By integrating molecular-level insights with mesoscale simulations, this research offers a framework for studying droplet formation and fluid instability. The results have significant implications for technologies such as nanotechnology manufacturing, microfluidics, and emulsification, paving the way for more efficient and controlled droplet-based systems.