A Mesoscale Study of Pinch-off under High Strain

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Abstract

We study the dynamic behavior of a pinching liquid thread as a function of the time to pinch-off. The novelty of this work resides in the use of a particle method (the Many-body Dissipative Particle Dynamics method, or MDPD), and in the inclusion of the interaction with a surrounding gas. As an MDPD calculation can be carried out at a scale below the continuity limit as a coarse-grained molecular simulation, this work represent a mesoscale approach to the study of spray formation.

Two issues are discussed in this paper. First, adding the effect of a second MDPD fluid requires the characterization of the friction interaction between particles of two immiscible fluids: unlike interfacial tension or solubility, this parameter does not have a directly related physical property. Second, in order to subject the liquid thread to a straining field, a two-phase, Non-Periodic Boundary Condition (NPBC) needs to be implemented. In the proposed NPBC method, two layers of particles are built into the domain on each side of the computational box. The outermost layer is modified at every iteration by placing particles of the prescribed type: this buffer works as a barrier whose composition depends on the instantaneous location of the boundary. The innermost layer contains thermalized particles that are otherwise free to move according to the distribution of the surrounding particles.

By enabling the simulation of pinch-off under extensional flow, an arbitrary strain rate can be imposed via the gas phase. The capillary number Ca therefore appears as an additional parameter controlling pinch-off, and the simulations illustrate the role of stochastic effects for a range of Ca values.

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