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Crossover behavior study of a thinning liquid bridge using the dissipative particle dynamics method

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ABSTRACT

In this work, the dissipative particle dynamics method is used to explore the thinning process of a liquid bridge transforming from macroscopic factor domination to thermal fluctuation domination. Both the inertial–force–dominated thinning profile and the thermal–fluctuation–dominated thinning profile are of self–similarity characteristics. Our simulations show that the scaling factors are in accordance with theoretical results. To explore crossover behavior, concentration is on the transitional regime, where both macroscopic factor domination and microscopic factor domination can be observed. The crossover time depends mainly on the stochastic coefficient. With the conservative forces not being considered, the decrease of the stochastic coefficient results in a wider thermal-fluctuation-dominated regime, but the crossover radius remains nearly unchanged. It is found that the increase in viscosity aids in the dominance of the thermal fluctuations and the emergence of the double–cone breakup profile. Surface stress fluctuations and bulk density fluctuations are examined to investigate the origin of the crossover. The results of these simulations suggest that the key factor of the crossover is the fluctuation correlation length, rather than the strength of the interfacial stress fluctuations. The simulation results also support the conclusion of previous researchers who have determined that it is the balance between the driving capillary pressure and the thermal energy density in the neck that causes crossover.

1. Introduction

A liquid bridge, or liquid thread tends to thin and breakup because of surface-tension-driven instability. The study of this event is of significant engineering and scientific importance because of the fundamental position of the droplet formation in many engineering applications such as atomization, spraying, fiber spinning, ink printing and many silicon chip technologies [1]. The singularity that forms as the fluid neck pinches off renders this problem very challenging. The self-similarity theory was typically used to investigate the nature of the singularity [1,2]. When the self-similarity is applied, the profile of the liquid bridge $h(z, t)$ can be written as:

$$h(z,t) = \frac{l_c}{t_c^{\alpha}}(t^* - t)^{\alpha} f\left(\frac{t_c^{\beta}}{l_c}\frac{z}{(t^* - t)^{\beta}}\right), \tag{1}$$

where $h(z, t)$ is the radius of the liquid bridge at axial coordinate z and time t, l_c is a fixed length scale $l_c = \eta^2/\rho\lambda$ and t_c is a fixed time scale $t_c = \eta^3/\rho\lambda^2$, with η, λ and ρ being respectively the shear viscosity, surface tension and liquid density. The function f is a universal similarity function. The variable t^* denotes the moment at which the liquid bridge breaks, α and β are scaling factors along the radial and axial directions, respectively. Various regimes with different dominating factors and scaling relationships have been identified by both theoretical and experimental analysis. Under the conditions of small viscosity, thinning is dominated by the interplay of surface tension and inertial forces, the scaling power α equals 2/3 [3,4]; so the neck radius $h(z_0, t)$ thins with $h_{\min}(t) \propto (t - t^*)^{2/3}$, where z_0 is the breakup position. And if the viscosity is large enough to have an effect, the scaling power α equals 1.0 [5]; so the neck radius will thin with $h_{\min}(t) \propto (t - t^*)$.

With the rapid development of nano technology, the thinning and breakup problem of a nanoscale liquid bridge is also gaining attention. It has been found that in nanoscale the thermal fluctuations will dominate. Theoretical analysis, molecular dynamics simulations and experiments all show that, in this situation, the scaling power will be 0.42; so the neck radius will thin with $h_{\min}(t) \propto (t - t^*)^{0.42}$ [6,7]. Thermal fluctuations also cause the thinning profile to take on a unique double-cone (DC) shape with the satellite droplet being effectively suppressed.

In general, the characteristics of a thinning liquid bridge dominated by the microscopic factor (thermal fluctuations) are very different from a bridge dominated by macroscopic factors

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(inertial force and viscosity). The problem of how the crossover from macroscopic-factor-dominated to thermal-fluctuation-dominated occurs remains to be solved [7]. A potential tool to investigate this problem is the molecular dynamics (MD) method. Given enough atoms and elapsed time, the MD simulation can imitate the entire thinning process, in which the radius of the liquid bridge is at first so large that it thins with the thermal fluctuations being negligible, then, with the radius becoming smaller, the thermal fluctuations inevitably begin to take effect. But this type of simulation will entail considerable computation resources. An alternative approach is to simulate the process with a mesoscopic method, such as dissipative particle dynamics.

Dissipative particle dynamics (DPD) is a coarse-grained method introduced by Hoogerbrugge and Koelman [8,9]. The particles in this model represent clusters of many atoms. It is neither molecular nor continuum, but it exhibits hydrodynamic behavior and has thermal fluctuations that can drive Brownian motions [10]. The DPD method and its derivation – the multi-body DPD have been used to investigate the instability problem of a liquid thread [11,12]. They are also able to quantitatively reproduce both the macroscopic–factor–dominated and thermal–fluctuation–dominated thinning process of a liquid bridge [13,14]; so it is reasonable to anticipate that the crossover behavior can be conveniently explored using this method. This research uses the DPD method to investigate the crossover behavior of a liquid bridge thinning from macroscopic–factor–domination to thermal-fluctuation-domination.

2. Methods

2.1. Dissipative particle dynamics

In the DPD method, every particle represents a cluster of atoms or a fluid region rather than a single atom. Pairwise random forces and dissipative forces are included in DPD to compensate for the excluded internal degrees of freedom inside particles. The total force $\mathbf{F}_{ij}$ between each pair of DPD particles is of the form:

$$\mathbf{F}_{ij} = \mathbf{F}^C_{ij} + \mathbf{F}^D_{ij} + \mathbf{F}^R_{ij}, \tag{2}$$

where $\mathbf{F}^C_{ij}$ is the conservative component, $\mathbf{F}^D_{ij}$ is the dissipative component and $\mathbf{F}^R_{ij}$ is the stochastic component. The conservative component is given by

$$\mathbf{F}^C_{ij} = \begin{cases} A\omega^C(r_{ij})\widehat{\mathbf{r}}_{ij} & r_{ij} < r^* \\ 0 & r_{ij} \geq r^* \end{cases}, \tag{3}$$

where $\widehat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$, r^* is the cutoff radius, $\omega^C(r_{ij})$ is often chosen to be $1 - r_{ij}/r^*$, rendering the conservative force a soft repulsive force; and A characterizes the strength of the force. The dissipative force is given by:

$$\mathbf{F}^D_{ij} = -\gamma\omega^D(r_{ij})(\widehat{\mathbf{r}}_{ij}\cdot\mathbf{v}_{ij})\widehat{\mathbf{r}}_{ij} \quad r_{ij} < r^*. \tag{4}$$

Here, $\mathbf{v}_{ij}$ is the relative velocity vector between atom i and atom j; the coefficient γ controls the strength of the dissipative force, and $\omega^D(r_{ij})$ characterizes the variation of the dissipative force with particle distance. The random force is:

$$\mathbf{F}^R_{ij} = \sigma\omega^R(r_{ij})\theta_{ij}\widehat{\mathbf{r}}_{ij} \quad r_{ij} < r^*, \tag{5}$$

where the σ denotes the strength of the random force, $\omega^R(r_{ij})$ is the weight function characterizing the variation of the random force with particle distance. θ_{ij} is the standard Gaussian noise. Español and Warren [15] have demonstrated that if the fluctuation–dissipative theorem is to be satisfied, the dissipative and stochastic components should be of the following relationships:

$$\omega^D(r_{ij}) = \left[\omega^R(r_{ij})\right]^2, \tag{6}$$

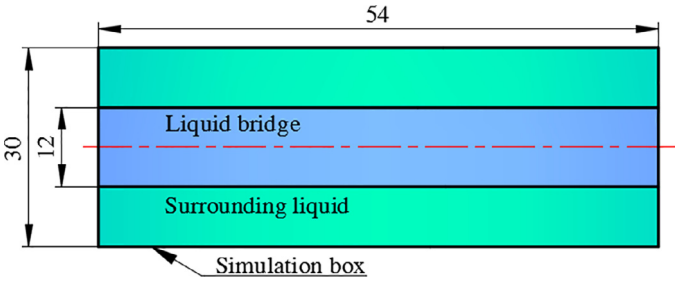

Fig. 1. Schematic of the simulation model. The simulation box is a slender cuboid with periodic boundary; the liquid bridge is positioned at the center surrounded by another liquid.

and

$$\sigma^2 = 2k_BT\gamma, \tag{7}$$

where k_B is the Boltzmann constant, and T is the temperature. This study uses a simple and common form of $\omega^D(r_{ij})$:

$$\omega^D(r_{ij}) = \begin{cases} \left(1 - r_{ij}/r^*\right)^s & r_{ij} < r^* \\ 0 & r_{ij} \geq r^* \end{cases}, \tag{8}$$

where the exponent s is typically set to be 2 or 1/2. The classic code LAMMPS [16] is used to perform simulations here.

Throughout this article we set the particle mass $m = 1$, the cutoff radius $r^* = 1$, and the characteristic energy $k_BT = 1$ to fix the units of mass, length, energy, and time, therefore most quantities in this article have been non-dimensionalized and are used without explicit units.

2.2. Simulation model

The simulation model used here is illustrated in Fig. 1; it is a periodic liquid bridge surrounded by another liquid. All the boundaries are periodic. In DPD, the flow near a solid wall boundary has many parametric dependencies on the wall [17]; and because of the soft potential in the DPD algorithm it is difficult to model a no–slip wall condition [18]. It is unnecessary to use solid wall boundaries in our simulations since the focus is only on the flow field near the breakup point, and the influence of solid boundaries is undesirable. For this reason, the choice was made to use periodic boundaries in all three directions of the simulation box. The simulation box is full of particles. Those particles belonging to the liquid bridge and those belonging to the surrounding liquid are distinguished by the heterogeneous conservative force coefficient: $A := A_{bb} = A_{ss}$, $A \neq A_{bs}$, where b has been used to denote the liquid bridge, and s the surrounding liquid. To simplify the model, other coefficients are identical: $\sigma := \sigma_{bb} = \sigma_{ss} = \sigma_{bs}$, $\gamma := \gamma_{bb} = \gamma_{bb} = \gamma_{bs}$. The standard DPD method can only simulate a system of homogeneous temperature; therefore this system does not consider thermal flux. The density is also homogeneous, so the bridge and the surrounding liquid are immiscible, but of the same dynamic properties. It can be seen from Fig. 1 that the initial radius of the liquid bridge is $R_0 = 6$ and the length is $L_z = 54$. This length is determined by ensuring that it is larger than the wavelength of the most unstable disturbance whose non–dimensional wave number is assumed to be $k' = kR_0 = 0.697$, according to Weber's formula [1]. To save computation time, at the initial stage a disturbance with $k' = 0.697$ is imposed on the liquid bridge to start the thinning of the liquid bridge. The transverse width of the simulation box is $L_x = L_y = 30$. Since periodic boundaries are used, there may be a finite size effect if the initial radius of the liquid bridge is a significant fraction of the simulation box size. To verify that the box is large enough, additional simulations were performed with a smaller box size ($L_x = L_y = 25$) to measure the growth rate of