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Investigation of temperature increase associated with liquid deformations at the nanometer scale

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HIGHLIGHTS

- Temperature increase due to film rupturing is derived using the molecular kinetic theory.
- The contribution of the molecular potential of a real fluid is considered.
- The approach is generalized to calculate the temperature increase in polyatomic molecules.
- The temperature increase in thread retraction is also estimated.

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ABSTRACT

The bursting of thin liquid films has been investigated for over a century. Recently, the velocity field and heat generation process in a rupturing film were clarified by numerical studies. In the present study, we discuss the temperature increase due to heat generation in a rupturing film on the basis of the molecular kinetic theory on a microcanonical ensemble, and we estimate the value of the temperature increase. We attempted to generalize the approach for calculating the temperature increase in polyatomic molecules. In addition, we applied the calculation to thread retraction and derived the value of the temperature increase due to heat generation in the system.

1. Introduction

The rupture of thin liquid films has been investigated for over a century [1,2]. Near the edge of a rupturing film, small droplets are ejected by the film [3,4], and surfactants are accumulated at the liquid rim [5,6]. Understanding such interfacial phenomena is crucial [7,8] in industrial and scientific fields such as atomization, spray, and foam technologies that are crucial in applications such as diesel engines, ink-jet printers, and metal foams. Although there are many capillary phenomena such as droplet wetting and dewetting of thin films, and capillary action, we focus on liquid/vapor systems, e.g., film rupturing and thread retraction, for simplicity. The non-equilibrium liquid interface of a rupturing liquid film is spontaneously deformed by the interfacial tension to minimize the interfacial energy. The interfacial energy that disappears in the process is converted to kinetic and thermal energy on approaching an equilibrium state [9,10].

The temperature increase due to film rupturing had not been considered in previous works. The kinetics of rupturing films was first discussed by Culick [11], who derived the following energy conservation equation based on the momentum

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conservation of the rupturing liquid film to theoretically obtain the rupturing velocity by assuming that the difference in the interface energy is distributed as both kinetic and viscous energies.

$$\gamma \Delta A = \frac{1}{2} M V^2 + Q, \tag{1}$$

where γ is the liquid/vapor surface tension, ΔA is the ruptured surface area, M is the mass of the ruptured region, V is the rupturing velocity, and Q is the thermal energy. Here, the thermal energy is equal to the kinetic energy [11], which was confirmed using a numerical simulation [12]. Culick predicted the value of the temperature increase by assuming that the entire rim of the rupturing liquid film is heated. Culick reported that in this case, when the film has a micrometer-scale thickness, the predicted temperature increase is on the order of 10^{-3} K, which is negligible [11].

For the rupture of a nanometer-scale thin film [13], the predicted temperature increase is on the order of 10^0 K; such an increase in temperature was observed in recently reported molecular dynamics simulations [14,15] because, in such a case, the heat capacity is too low and the rupturing velocity is much higher compared to a film of micrometer-scale thickness. The temperature increase would result in variations of the properties, e.g. surface tension and density that have high temperature dependences [16], and the liquid deformation process would consequently become complicated.

Therefore, in the case of a nanometer-scale system [14], it is important to understand liquid deformations such as film rupturing and thread retraction by taking the temperature variation into account. In the present study, we demonstrate the derivation of the temperature increase due to film rupturing by using the energy conservation of the film rupturing from the perspective of the molecular kinetic theory. In addition, we applied the approach to derive the temperature increase due to thread retraction.

2. Moving interface speed

The rupturing velocity of a thin liquid film (F) was derived by Taylor [17] and Culick [11], who used the equation of motion and energy conservation, respectively, to obtain the following relation:

$$V_{\mathrm{F}} = \sqrt{\frac{2\gamma}{\rho e_0}}, \tag{2}$$

where V_{F} is the rupturing velocity of thin liquid film, ρ is the density, and e_0 is the initial film thickness. This rupturing velocity is called as Taylor–Culick speed, which is found in any viscosity conditions [18–20]. Although the state of the rupturing film is determined by the balance between viscous, capillary, and inertial effects, in the present study, we focus on the inertial state, which is dominant because of the rupturing shape; the mass of the ruptured region is expected to correspond to the generated heat. By neglecting the additional curvature in the radial direction of a liquid cylinder, the above discussion on film rupturing can be applied to liquid thread retraction (T), which can have an equation of motion similar to that in the case of film rupturing. The velocity of the moving interface can be estimated as [21]:

$$V_{\mathrm{T}} = \sqrt{\frac{2\gamma}{\rho R_{\mathrm{T}}}}, \tag{3}$$

where R_{T} is the radius of a thread shown in Fig. 1(b). The predicted moving interface speed in Eq. (3) has been qualitatively observed in a previous experiment [22]. In the case of the liquid thread retraction, it has been reported that the velocity of a jet from a nozzle has to be larger than a threshold value so that the jet is ejected from the outlet, which implies that the thread of the jet should have a high retracting speed [23]. Thread retraction toward an opposite jet direction has also been reported for the jet of a viscoelastic liquid, which was discussed qualitatively with the factor 2 removed from Eq. (3) [24]. In the present study, we estimate the value of the temperature increase due to the heat generation by assuming that the moving interface speeds converge to the velocities in (2)–(3) in the case of the above deformations.

3. Energy conservation from molecular kinetic theory

Considering the systems as microcanonical ensembles, the Hamiltonian H remains constant with time t [25] as follows because of energy conservation:

$$H(0) = H(t). \tag{4}$$

As the Hamiltonian is the sum of kinetic energy E_k and potential energy E_p, Eq. (4) can be expressed as,

$$E_p(0) + E_k(0) = E_p(t) + E_k(t). \tag{5}$$

In the case of a monatomic molecule, the temperature is defined by the translational kinetic energy, neglecting both the rotational kinetic energy and vibrational kinetic energy, as follows:

$$\frac{3}{2} k_{\mathrm{B}} N T = \sum \frac{1}{2} m_i \boldsymbol{v}_i^2, \tag{6}$$