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Editor's Choice

Droplet evaporation on a horizontal substrate under gravity field by mesoscopic modeling

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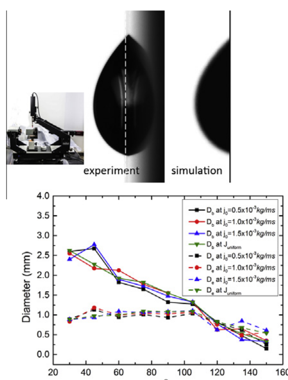
HIGHLIGHTS

- A novel evaporation scheme introduced to the multiphase LBM model for the numerical framework.
- A new method proposed to determine the critical drop size of gravity effect.
- Critical diameter of water drop is independent of evaporation conditions, and surface wettability for normal cases.

GRAPHICAL ABSTRACT



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ABSTRACT

The evaporation of water drop deposited on a horizontal substrate is investigated using a lattice Boltzmann method (LBM) for multiphase flows with a large-density ratio. To account for the variation of evaporation flux distribution along the drop interface, a novel evaporation scheme is introduced into the LBM framework, and validated by comparison with experimental data. We aim at discovering the effect of gravity on the evaporating drop in detail, and various evaporation conditions are considered as well as different wetting properties of the substrates. An effective diameter is introduced as an indicator of the critical drop size under which gravity is negligible. Our results show that such critical diameter is much smaller than the capillary length, which has been widely accepted as the critical size in previous and current works. The critical diameter is found to be almost independent of the evaporation conditions and the surface wettability. A correlation between this critical diameter and the capillary length is also proposed for easy use in applications.

1. Introduction

Evaporation of a liquid drop on a solid substrate is a common phenomenon in everyday life, such as inkjet printing [1], accidental drippings on a hot surface [2], and the well-known "coffee-stain" effect [3–5]. As recent applications such as particle synthesis [6], DNA/RNA arrangement [7] and medical diagnostics [8] emerge, this phenomenon has gained more and more attention.

The evaporation process has been extensively discussed [9], including the shape morphology, the evaporation flux distribution and the internal flow patterns of drops. For a pure sessile droplet, there are three evaporation modes [10–13]: constant contact area (contact line pinning) mode, constant contact angle mode, and

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both-changing mode. Along with this, evolution rules of contact angle and contact diameter or other shape properties were investigated for hydrophilic [14–20] or hydrophobic [21–26] surfaces. As for the spatial distribution of the evaporation flux, an enhancement near the contact edge was predicted for a hydrophilic drop by theoretical models [3,5,27] and numerical simulations [28–33], which is also confirmed by some experimental measurements [34–36]. In addition, the flow pattern inside drops was found to be strongly interrelated with the evaporation flux [37,38]. Most of these studies considered drops of smaller size than the capillary length, $L_c = \sqrt{\sigma/(\rho_L f_g)}$, (2.7 mm for water droplets), where σ is the surface tension, ρ_L the liquid density and f_g the gravity acceleration, hence the gravity effect was assumed to be negligible [21,39]. However, since the capillary length is usually calculated using properties at equilibrium, it may not be entirely appropriate in case of a strongly non-equilibrium process such as drop evaporation.

This work aims to reveal the impact of gravity on drop evaporation by mesoscopic modeling. In the last two decades, the lattice Boltzmann method (LBM) has become a powerful numerical scheme for fluid flow because of its advantages in dealing efficiently with complicated boundaries and interfacial transport dynamics [40–43]. Various LBM models have been developed for multiphase hydrodynamics, including the color-fluid model proposed by Gunstensen et al. [44,45], the pseudo-potential model proposed by Shan and Chen [46,47], the free-energy model by Swift et al. [48] and the mean-field model by He et al. [49,50]. Although these methods worked for some cases, they suffered from numerical instabilities for large density ratio and large viscosity ratio. Consequently, two types of models for large density ratio were developed by Zheng et al. [51] and Inamuro et al. [52,53] respectively. Both models improved the capability to deal with density ratios up to 1000 or more. It was reported that Zheng's model was more efficient and easy to implement than the Inamuro's model, and the latter met some challenges for incompressible flows [51]. Very recently, a few LBM studies [54–56] have focused on evaporation; however, the evaporation flux under gravity has never been investigated so far.

In this work, we study the evaporation of water drops deposited on a horizontal substrate by LBM simulations with special focus on the effects of gravity. We develop a numerical approach within the framework of LBM to account for evaporation regularities. After validation, the steady-state drop shapes at different scales under gravity are compared for different drop wettabilities and different evaporation modes. We introduce a critical characteristic diameter during evaporation under gravity to determine when gravity effects become significant, in alternative to the standard capillary length.

2. Numerical methods

2.1. The multiphase LBM model

The LBM model based on the free-energy scheme is adopted in this work proposed by Zheng et al. [51] for multiphase flows with large density ratios. Here, we will briefly introduce the main scheme of this model. Two distribution functions f_i and g_i are introduced to account for hydrodynamics and interfacial dynamics, respectively. The evolution equations are given as

$$f_i(\boldsymbol{x}+\mathbf{c_i}\Delta t, t+\Delta t) - f_i(\boldsymbol{x},t) = -\frac{1}{\tau_f}\left(f_i(\boldsymbol{x},t) - f_i^{eq}(\boldsymbol{x},t)\right) + \frac{3\Delta t\omega_i \mathbf{c_{i\alpha}}(\mu\partial_\alpha\phi + n\mathbf{G})}{c^2}, \quad (1)$$

$$g_i(\boldsymbol{x}+\mathbf{c_i}\Delta t, t+\Delta t) - g_i(\boldsymbol{x},t) = -\frac{1}{\tau_g}\left(g_i(\boldsymbol{x},t) - g_i^{eq}(\boldsymbol{x},t)\right), \quad (2)$$

where the subscript α is for the spatial coordinates, i is the direction of discrete velocities $\mathbf{c_i}$; ω_i is the related weight coefficient, Δt is the time step, τ_f and τ_g are the relaxation times; the macroscopic variable $\mathbf{G}$ is the acceleration of body force, $n = \frac{\rho_A+\rho_B}{2}$ is the average density, $\phi = \frac{\rho_A-\rho_B}{2}$ is the order parameter to distinguish phases A and B with density ρ_A and ρ_B respectively; μ is the chemical potential with the expression of

$$\mu = a(4\phi^3 - 4\phi^{*2}\phi) - \kappa\Delta\phi, \quad (3)$$

where ϕ^* is the maximum order parameter. The term $\mu\partial_\alpha\phi$ in Eq. (1) correlates to the Laplace pressure caused by interface actions. a and κ are two coefficients related to the interface tension σ as

$$a = (3\sigma)/(4W\phi^{*4}), \quad (4)$$

$$\kappa = (3\sigma W)/(8\phi^{*2}), \quad (5)$$

where W is the interface width.

By using the Chapman–Enskog expansion, Eqs. (1) and (2) can recover the Navier–Stokes equation and the convective Cahn–Hilliard equation [57] at a second-order accuracy. Noticing that the convective Cahn–Hilliard equation $(\partial_t\phi + (\boldsymbol{u}\cdot\nabla)\phi = M\nabla^2\mu)$ is used for interface capturing and can describe flows with large density ratios well, Zheng's model can deal with large-density-ratio multiphase flows successfully.

2.2. Evaporation flux distribution

Consider a sessile drop evaporating on a horizontal substrate, as shown in Fig. 1. The evaporation flux rate along the droplet surface is the first concern for studies of microscopic behavior of drop evaporation. A uniform evaporation flux rate at the liquid–gas interface is the easiest and straightforward assumption, but it is not valid for most cases. Based on molecular kinetic theories and other capillary theories, there is a general consensus about the main features of the evaporation flux and its dependence on the position, which are summarized in Ref. [39].

When $\theta < 90°$, the local evaporation mass flux $J(r,t)$ is not uniform and a widely used correlation was given by Hu and Larson [28] as

$$J(r,t) = j_0\frac{g(\theta)}{R}\left(1-\left(\frac{r}{R}\right)^2\right)^{-\lambda} \quad \lambda = \frac{\pi-2\theta}{2\pi-2\theta} \quad (6a)$$

$$g(\theta) = (0.27\theta^2+1.30)\left(0.6381-0.2239\left(\theta-\frac{\pi}{4}\right)^2\right), \quad (6b)$$

where j_0 is the evaporation parameter, related to the vapor diffusivity D (m^2/s), the saturated vapor concentration c_V (kg/m^3), and the relative humidity H as

$$j_0 = Dc_V(1-H). \quad (6c)$$

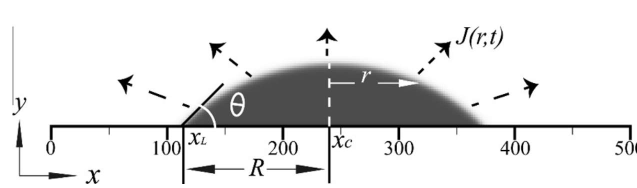

Fig. 1. Physical model of a sessile droplet evaporating on a horizontal substrate. θ is the contact angle, R is the base radius, r is the distance to the drop axis, x_c is the coordinate of droplet center, x_L is the coordinate of contact line on the left edge, and $J(r,t)$ is the local evaporation mass flux.