A sharp-interface level-set method for analysis of Marangoni effect on microdroplet evaporation ☆

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ABSTRACT

A level-set method is presented for computation of microdroplet evaporation including not only the effects of heat and mass transfer, phase change and contact line dynamics but also the Marangoni effect, which is a key parameter affecting the internal flow of the droplet and the particle deposition pattern. A sharp-interface formulation of the Marangoni force is derived and tested for two-phase Marangoni convection in a cavity. The computed results show good convergence in both the liquid and gas regions and are in excellent agreement with the analytical solutions. The level-set formulation is applied to microdroplet evaporation on a solid surface to investigate the Marangoni effect.

1. Introduction

Microdroplet evaporation on a solid surface is an integral process for inkjet fabrication of various microstructures [1,2]. Despite extensive experimental and theoretical studies of the evaporation process [2–4], its general predictive model has not yet been developed due to the complexity of the associated interfacial flow including heat and mass transfer, phase change and contact line dynamics.

Recently, numerical simulations for more general analysis of droplet evaporation were performed in several studies using a body-fitted moving-grid method [5] and a finite element method (FEM) [6–10]. The Lagrangian methods are generally not easy to extend to the interface configurations with large distortion or change in topology. Such difficulties can be overcome by employing Eulerian methods such as the volume-of-fluid (VOF) method and a level-set (LS) method.

Briones et al. [11,12] computed droplet impact and evaporation using the explicit VOF method in the commercial CFD code FLUENT. The VOF method was modified to include the effect of evaporation at the interface. However, the interface conditions for the coupled vapor concentration, temperature and evaporation flux are not easy to implement in the VOF method. Tanguy et al. [13] developed the LS method for computation of droplet evaporation combining with the ghost fluid approach to accurately implement the interface conditions. Son [14,15] extended the LS method to droplet impact and evaporation on a solid surface by including a dynamic contact angle model.

In this work, the LS formulation is extended for analysis of microdroplet evaporation including the Marangoni effect, which can change the internal flow of the droplet and thus control the particle deposition pattern [16]. The Marangoni effect can be easily formulated in a body-fitted moving-grid method [5] and a FEM [7–9], where the interface coincides with the grid points, but it is not so straightforward to accurately implement in the Eulerian methods. A sharp-interface formulation of the Marangoni force is presented and compared with the delta function formulation employed in the VOF method [17–19] and the LS method [20,21]. The sharp-interface LS formulation is tested through computation of two-phase Marangoni convection in a cavity, whose analytical solution is available in the literature [22], and droplet evaporation on a solid surface.

2. Numerical analysis

The present numerical approach is based on the sharp-interface LS formulation developed by Son and Dhir [23] for film boiling and Son [14,15] for droplet evaporation. The LS method is extended for analysis of the Marangoni effect on microdroplet evaporation. The droplet surface is tracked by the LS function ϕ, which is defined as a signed distance from the interface. The negative sign is chosen for the gas phase and the positive sign for the liquid phase. In this work, the following assumptions are made: (1) the gas phase is an ideal mixture of air and vapor; (2) the liquid phase is a pure substance; (3) the interface temperature is below the boiling temperature; and (4) the effect of gravity is negligible while considering the microscale droplet motion.

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Nomenclature

c	specific heat
D_c	droplet–wall contact diameter
D_v	diffusion coefficient of vapor in air
F_l	fraction function
h	grid spacing
h_{lg}	latent heat of vaporization
H	height
L	domain width
$\dot{m}$	mass flux across the interface
M	molecular mass
$\mathbf{n}$	unit normal vector
p	pressure
r,y	cylindrical coordinates
R	droplet radius
S	sign function
t	time
T	temperature
$\mathbf{u}$	flow velocity vector
$\mathbf{U}$	interface velocity vector
Y_v	vapor mass fraction

Greek symbols

α	step function
β	difference between the liquid and gas specific volumes
θ_a	advancing contact angle
θ_r	receding contact angle
κ	interface curvature
λ	thermal conductivity
μ	dynamic viscosity
ρ	density
σ	surface tension coefficient
τ	artificial time
ϕ	distance function from the liquid–gas interface

Subscripts

a,v	air, vapor
g,l	gas, liquid
I	interface
o	initial
sat	saturation
w	wall

Superscripts

$\wedge$	effective property
$*$	intermediate step

2.1. Governing equations

The conservation equations of mass, momentum and energy for each phase, and the vapor mass fraction Y_v for the gas phase are expressed as

$$\nabla \cdot \mathbf{u}_f = 0 \tag{1}$$

$$\rho_f\left(\frac{\partial \mathbf{u}_f}{\partial t} + \mathbf{u}_f \cdot \nabla \mathbf{u}_f\right) = -(\nabla p)_f + \nabla \cdot \mu_f\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)_f \tag{2}$$

$$\rho_f c_f\left(\frac{\partial T_f}{\partial t} + \mathbf{u}_f \cdot \nabla T_f\right) = \nabla \cdot \lambda_f(\nabla T)_f \tag{3}$$

$$\frac{\partial Y_v}{\partial t} + \mathbf{u}_g \cdot \nabla Y_v = \nabla \cdot D_v(\nabla Y_v)_g \tag{4}$$

where the subscript f denotes the liquid phase (l) for $\phi > 0$ and the gas phase (g) for $\phi \leq 0$. The conservation equations for each phase are coupled through the matching (or boundary) conditions at the interface ($\phi = 0$):

$$\mathbf{u}_l - \mathbf{u}_g = \beta \dot{m}\mathbf{n} \tag{5}$$

$$\mathbf{n} \cdot \left[\left(p_g - p_l\right)\mathbf{I} + \mu_l\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)_l - \mu_g\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)_g\right]$$
$$= \left(\sigma\kappa - \beta \dot{m}^2\right)\mathbf{n} - \nabla_s \sigma \tag{6}$$

$$T_f = T_I \tag{7}$$

$$Y_v = Y_{v,I} \tag{8}$$

where $\beta = \rho_g^{-1} - \rho_l^{-1}$ and the surface tension coefficient can be expressed as a function of interface temperature

$$\sigma = \sigma_{ref} - |\sigma_T|\left(T - T_{ref}\right). \tag{9}$$

The Marangoni stress due to the gradient of surface tension coefficient can be rewritten as

$$\nabla_s \sigma = \nabla \sigma - \mathbf{n}(\mathbf{n} \cdot \nabla \sigma) \tag{10}$$

where it is noted that $\mathbf{n} \cdot \nabla_s \sigma = 0$. The interface normal $\mathbf{n}$, the interface curvature κ, and the evaporative mass flux $\dot{m}$ are defined as

$$\mathbf{n} = \nabla \phi / |\nabla \phi| \tag{11}$$

$$\kappa = \nabla \cdot \mathbf{n} \tag{12}$$

$$\dot{m} = \rho_f\left(\mathbf{U} - \mathbf{u}_f\right) \cdot \mathbf{n} \tag{13}$$

where $\mathbf{U}$ is the interface velocity. T_I, $Y_{v,I}$, and $\dot{m}$ can be evaluated from the following coupled equations for the mass and energy balances at the interface and the thermodynamic relation, as done in Ref. [14]

$$\dot{m} = \frac{\mathbf{n} \cdot \rho_g D_v \nabla Y_{vg}}{1 - Y_{v,I}} = \frac{\mathbf{n} \cdot \left[\lambda_l(\nabla T)_l - \lambda_g(\nabla T)_g\right]}{h_{lg}} \tag{14}$$

$$Y_{v,I} = \frac{M_v p_{v,sat}(T_I)}{M_v p_{v,sat}(T_I) + M_a\left[p_\infty - p_{v,sat}(T_I)\right]}. \tag{15}$$

Based on the ghost fluid method (GFM) [24–26], which is a numerical technique for accurately enforcing the boundary conditions at the interface without being smoothed over several grid spacings, the conservation equations can be rewritten for the liquid–gas region as [14,15,23]

$$\nabla \cdot \mathbf{u} = \beta \dot{m}\mathbf{n} \cdot \nabla \alpha \tag{16}$$