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Numerical simulation of stick-slip contact line motion and particle line formation in dip coating☆

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ABSTRACT

Numerical simulation is performed for stick-slip contact line motion and particle line formation in dip coating. The liquid–gas interface as well as the liquid–gas–solid contact line is tracked by a sharp-interface level-set method, which is extended to include the effect of phase change, to implement the contact angle model for the stick-slip contact line motion, and to treat the particle deposition on a moving substrate. The computations demonstrate that the particle line formation is directly related to the stick-slip contact line motion. The effects of initial particle concentration, substrate withdrawal velocity, substrate temperature and contact angle on the particle line formation in dip coating are investigated.

1. Introduction

Dip coating in the evaporation regime, where a substrate is slowly pulled up from an evaporating liquid pool, has received considerable attention as a simple particle deposition process for patterning of microscale stripes or lines. The particle line patterning is related to the periodic stick-slip motion of the liquid–gas–solid contact line, as optically observed in several studies [1-5]. However, a fundamental understanding and prediction of the stick-slip contact line motion and the associated particle line deposition process is lacking in the literature.

Ghosh et al. [6] conducted experiments for line patterning by dip coating of colloidal particles and showed that periodic particle lines form spontaneously at the liquid–gas–solid contact line. In a low velocity regime of substrate withdrawal, the line width and spacing are almost independent of the substrate velocity. However, when the substrate reaches a critical velocity, the line width and spacing are reduced significantly. This transition of line patterning was assumed to occur when the liquid film thickness is below the particle size. More comprehensive experiments for particle line patterning were carried out by Watanabe et al. [7] considering the effects of particle concentration, evaporation rate as well as substrate velocity V_w. Their data showed that the line width increases linearly with the particle concentration and varies as $V_w^{-0.8}$ or V_w^{-1}, but the line spacing does not depend on the particle concentration and the substrate velocity. The evaporation rate has little influence on the line width and spacing. They proposed a new mechanism for particle line formation based on a curved shape of the liquid–gas interface. Berteloot et al. [8] measured the weight of particle deposit in dip coating for various substrate velocities and showed that the mean thickness of the deposit varies as V_w^{-1} in the evaporation regime whereas it varies as $V_w^{2/3}$ in a higher velocity (or Landau–Levich) regime of the substrate.

As an alternative way to further clarify the dip coating process, numerical simulation of two-phase flows driven by a moving substrate was performed by several researchers [9-11]. However, their analysis did not include the effects of liquid evaporation and particle deposition. Such effects were investigated in numerical studies of sessile droplet evaporation and particle deposition using body-fitted moving-grid methods [12,13], finite elements methods [14-19], lubrication approximation methods [20,21], a volume-of-fluid method [22] and a level-set (LS) method [23-28]. Very recently, Lee and Son [29,30] developed the LS method for analysis of liquid evaporation and particle deposition in dip coating. While solving an advection–diffusion equation for particle concentration, they used a first-order rate formulation [17,31] as a boundary condition for the particle deposition on the substrate.

In this work, the LS method is further extended for computation of the stick-slip contact line motion and particle line pattering in dip coating. Numerical techniques are developed for implementation of the dynamic behavior of liquid–gas–solid contact line on a moving substrate and the associated particle deposition. The effects of initial particle concentration, substrate withdrawal velocity, substrate temperature and contact angle on the particle line formation in dip coating are investigated.

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Nomenclature

c	specific heat
d_p	particle diameter
D_p	diffusion coefficient of particles in liquid
D_v	diffusion coefficient of vapor in air
F	fraction function
g	gravity
h	grid spacing
h_{lg}	latent heat of vaporization
H	height
k_d	particle deposition rate constant
L	length
M	molecular mass
$\dot{m}$	mass flux across the interface
$\mathbf{n}$	unit normal vector
p	pressure
t	time
T	temperature
$\mathbf{u}$	flow velocity vector, (u, v)
V_w	substrate withdrawal velocity
W_p	particle deposition thickness
x, y	Cartesian coordinates
Y_p	particle volume fraction
Y_v	vapor mass fraction

Greek symbols

α	step function
β	$\rho_g^{-1} - \rho_l^{-1}$
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
f	fluid
g, l	gas, liquid
I	interface
o	initial
p	particle
sat	saturation
w	wall
∞	ambient

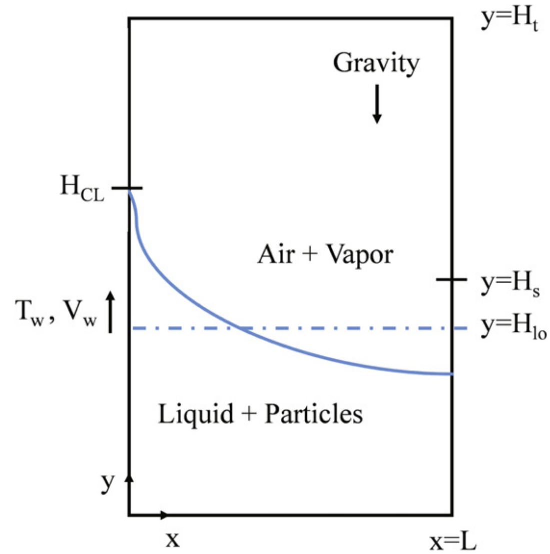

Fig. 1. Computational domain.

2. Numerical analysis

The present numerical approach is based on the sharp-interface LS formulation developed in our previous studies [29,30] for liquid evaporation and particle distribution. The LS method is extended for analysis of the stick-slip contact line motion and particle line formation in dip coating. The liquid–gas interface is tracked by the LS function ϕ, which is defined as a signed distance from the interface. The positive sign is chosen for the liquid phase and the negative sign for the gas phase. Fig. 1 shows the configuration used for computation of dip coating. In this work, the following assumptions are made: (1) The flow, temperature and concentration fields are two-dimensional; (2) the gas phase is an ideal mixture of air and vapor; (3) the liquid phase is a mixture of evaporating liquid and non-evaporating particles; and (4) the substrate temperature is below the boiling temperature.

The conservation equations of mass, momentum and energy in the liquid and gas phases, vapor mass fraction (Y_v) in the gas phase, and particle volume fraction (Y_p) in the liquid phase can be expressed as [29,30]

$$\nabla \cdot \mathbf{u} = \beta \dot{m} \mathbf{n} \cdot \nabla \alpha \tag{1}$$

$$\hat{\rho}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}_f \cdot \nabla \mathbf{u}_f\right) = -\left[\nabla p + \left(\sigma\kappa - \beta\dot{m}^2\right)\nabla\alpha\right] + \nabla \cdot \hat{\mu}\nabla\mathbf{u} + \mathbf{f} \tag{2}$$

$$(\hat{\rho c})\left(\frac{\partial T}{\partial t} + \mathbf{u}_f \cdot \nabla T\right) = \nabla \cdot \hat{\lambda}\nabla T \quad \text{if} \quad \phi \neq 0 \tag{3}$$

$$T = T_I \quad \text{if} \quad \phi = 0 \tag{4}$$

$$\frac{\partial Y_v}{\partial t} + \mathbf{u}_g \cdot \nabla Y_v = \nabla \cdot \hat{D}_v \nabla Y_v \quad \text{if} \quad \phi < 0 \tag{5}$$

$$Y_v = Y_{v,I} \quad \text{if} \quad \phi = 0 \tag{6}$$

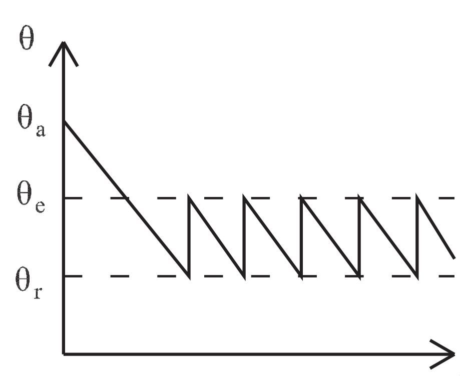

Fig. 2. Schematic of contact angle variation in the stick-slip contact line motion.