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Numerical study and predictions of evolution behaviors of evaporating pinned droplets based on a comprehensive model

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ABSTRACT

In this paper, an evaporation model, which comprehensively considers transport mechanisms that include vapor diffusion in air, evaporative cooling at liquid–air interface, conjugate heat transfer in solid, liquid and air, buoyancy-induced convection and Marangoni convection in both liquid and air, is established to study the evaporation of pinned droplets on both unheated and heated substrates. Based on this model and using the adaptive evolution algorithm proposed by the authors, the temporal evolution behaviors of pinned droplets are simulated. Numerical results show that the temporal evolutions of contact angle and volume of pinned droplets with an initial contact angle $\theta_0 = \pi/2$, when normalized, follow the same laws, respectively, though there exist great differences in the droplet base radius, substrate temperature and ambient humidity. From the numerical results, the simple normalized correlations for the temporal evolutions of contact angle and volume of pinned droplets with $\theta_0 = \pi/2$ are developed, and further, the general expressions in closed forms applicable for predicting the evolution behaviors of evaporating pinned droplets with $\theta_0 \leq \pi/2$ on both unheated and heated substrates are deduced by considering the evaporation process of droplets with $\theta_0 \leq \pi/2$ as a part of the evaporation process of droplets with $\theta_0 = \pi/2$. Finally, the proposed expressions are compared and validated with the theoretical and experimental results in the literature.

1. Introduction

The evaporation of sessile droplets has wide applications ranging from the industrial area such as spray cooling [1], coating technology [2], to the biochemistry area such as protein detection [3], DNA chip manufacture [4], etc. Generally, there occur two typical evaporation modes of sessile droplets: pinning mode and de-pinning mode [5]. In the pinning mode, the base radius of droplets keeps constant while the contact angle decreases. In the de-pinning mode, however, the contact angle of droplets keeps constant while the base radius decreases. In many practical applications, the pinning mode dominates the droplet evaporation process. For instance, the ring-like deposition (also known as coffee-ring) of colloidal dispersion droplets, which has been widely utilized in the bioassays etc. [4,6,7], is mainly induced by the pinned contact line in the pinning mode [8]. For the pinning mode, the evolutions of contact angle and volume of droplets with time have attracted considerable attention over the past decades [9].

Many experimental studies have been carried out on the evolutions of contact angle and volume (or mass) of pinned droplets with time [10–16]. Birdi and Vu [10] measured the weight of evaporating water droplets on an unheated glass substrate, and found that the droplet mass decreased almost linearly with time. Crafton and Black [11] captured the side-view images of pinned droplets on heated aluminum and copper substrates. Their results showed that both contact angle and droplet volume decreased nonlinearly with time. Sobac and Brutin [12] experimentally investigated the evaporating behavior of pinned droplets on both unheated and heated substrates, and indicated that the thermal-linked mechanisms (such as buoyancy-induced convection, evaporative cooling, etc.) became increasingly important in the temporal evolutions of contact angle and volume of droplets as the substrate temperature increased. Other experimental studies showed that the substrate material properties [13], ambient air conditions [14] also influenced the evolution process of pinned droplets. As seen above, though various factors influencing the

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Nomenclature

c	vapor concentration [kg m^{-3}]
c_{sat}	saturated vapor concentration [kg m^{-3}]
D	diffusivity of water vapor in air [m^2 s^{-1}]
g	gravity constant [m s^{-2}]
h	height of droplet surface [m]
h_{vap}	latent heat of vaporization [J kg^{-1}]
H	relative humidity of air
J	local evaporation flux [kg s^{-1} m^{-2}]
k	thermal conductivity [W m^{-1} K^{-1}]
l_c	$=\sqrt{\sigma/\rho g}$ capillary length [m]
L	size of computation domain [m]
L_w	thickness of substrate [m]
$\overline{M}$	molar weight [kg mol^{-1}]
$\boldsymbol{n}_{l,a}$	unit vector in the normal direction
p	pressure [N m^{-2}]
r	radial coordinate [m]
R	base radius [m]
$\overline{R}$	universal gas constant [J mol^{-1} K^{-1}]
R_w	radius of substrate [m]
t	time [s]
t_{conv}	time scale for convection [s]
t_{cross}	time scale for crossing the interface [s]
t_{diff}	time scale for diffusion [s]
t_f	droplet lifetime [s]
t_{ht}	time scale for heat transfer [s]
$\boldsymbol{t}_{l,a}$	unit vector in the tangential direction
T	temperature [°C]
T_w	temperature of substrate bottom [°C]
T_∞	temperature of far field [°C]
$\boldsymbol{u}$	$=(u, v)$ velocity vector [m s^{-1}]
u	radial component of velocity vector [m s^{-1}]
U	characteristic velocity [m s^{-1}]
v	axial component of velocity vector [m s^{-1}]
V	droplet volume [m^3]
$\dot{V}$	volume evaporation rate [m^3 s^{-1}]
z	vertical coordinate [m]

Greek symbols

α	$=k/\rho c_p$ thermal diffusivity [m^2 s^{-1}]
β_l	thermal expansivity of liquid [K^{-1}]
θ	contact angle
ε	mesh-independence criterion
μ	dynamic viscosity [N s m^{-2}]
ρ	density [kg m^{-3}]
σ	surface tension [N m^{-1}]
τ	viscous stress [N m^{-2}]
ξ_n	convergence criterion for adaptive evolution algorithm

Subscript

0	initial
a	air
f	final
l	liquid
s	solid
v	vapor
w	substrate wall
n	serial number of computation step
∞	far field

Superscript

*	non-dimensional

evolution process of pinned droplets can be revealed by experimental studies, the exact expressions for predicting the evolutions of volume and contact angle of pinned droplets with time are difficult to be obtained experimentally.

Therefore, theoretical and numerical endeavors have been made on the prediction of evolution behaviors of pinned droplets. Hu and Larson [17] numerically simulated the temporal evolution of volume of pinned droplets on an unheated substrate based on the diffusion-driven model [5,18], in which the droplet evaporation is assumed to be isothermal and driven purely by vapor diffusion that can be described by the Laplace equation. From the numerical results, they developed a well-accepted correlation for the evaporation rate of sessile droplets as a function of contact angle (i.e. $dV/dt \sim \theta$), however, the expressions for the evolutions of droplet volume and contact angle with time cannot be deduced from this correlation. Subsequently, Popov [19] solved analytically the Laplace equation, and derived a non-closed expression for the evaporation rate of sessile droplets. Based on Popov's work, Sobac & Brutin [20] and Gelderblom et al. [21] deduced the dimensionless differential equations of mass and contact angle of pinned droplets with time on an unheated substrate. With the same pure diffusion-driven model, Semenov et al. [22] developed analytically a non-closed dimensionless expression for the temporal evolution of contact angle of pinned droplets, which needs a further numerical computation. Note that the pure diffusion-driven model used in above literature is only feasible for the situations where both thermal and convection effects can be negligible [23]. In fact, for most practical evaporation processes of sessile droplets, effects of thermal and convection need to be considered, especially for droplets evaporating on heated substrates [24]. Thus, Dunn et al. [25] improved the diffusion-driven model by considering evaporative cooling and thermal conduction in liquid droplet and solid substrate (i.e. the conduction-diffusion model). They numerically simulated the evolution of volume with time for pinned droplets, and found the simulation results deviated from the experimental results for water droplets, which they attributed to the neglect of natural convection in air in their model [26]. Incorporating the natural convection and heat transfer in air into the model of Dunn et al. [25], Saada et al. [27] simulated the evolution of pinned droplets on both unheated and heated substrates. Their model showed a better agreement with the experimental data than the conduction-diffusion model, but the convection in liquid was still ignored in their model, also no expression for predicting the evolution of pinned droplets was provided. Girard et al. [28] numerically studied the evolution of pinned droplets on heated substrates by considering the Marangoni convection in liquid while ignoring the natural convection in air in their model. From the numerical results, they developed an empirical expression for predicting the lifetime of pinned droplets on heated substrates, but the expressions for predicting the evolutions of contact angle and volume of pinned droplets on heated substrates were still absent in their work.

As reviewed above, though great progress has been made on the prediction of evolution behaviors of evaporating pinned droplets, there exist two main problems that need to be solved: (1) the evaporation of pinned droplets is a complex process governed by