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Transient effects and mass convection in sessile droplet evaporation: The role of liquid and substrate thermophysical properties

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ABSTRACT

In this paper, a transient droplet evaporation model based on Arbitrary Lagrangian–Eulerian (ALE) frame, which tracks the liquid-gas interface evolution and fully couples heat and mass transfer in solid, liquid and gas domains, was used to study the spontaneous evaporation of water, methanol and 3MP droplet (with low to high volatility) on PTFE substrates with small thermal conductivities and Al substrates with large thermal conductivities. It was found that because of the fully coupled transportation processes in droplet evaporation, the duration of transient periods determined according to the judgment criterion based on whether droplet or substrate are very close to each other. The larger the droplet volatility and the smaller the substrate thermal diffusivity, the longer the period of transient stage (normalized) of droplet evaporation, with 33.3% of the droplet lifetime for 3MP on a PTFE substrate. The larger the volatility and the substrate thermal conductivity, the larger the contribution of convective mass transfer for total evaporation, with the under-predictions of diffusive model of 41% for 3MP droplet on Al substrates. The percentage of contribution of natural convection is 29–64% of total contribution of convective mass transport, which points out the necessity of considering natural convection in the modelling of convective mass transfer. The main characteristics of flow field with and without buoyancy flow under the different combination of substrate and liquid material and their roles on mass transfer are discussed.

1. Introduction

Evaporation of a sessile droplet on a substrate is fundamental for widespread important applications, such as DNA micro array analysis, thin film coating, ink-jet printing, and spray cooling. Excellent overviews on literatures on sessile droplet evaporation have been given by Cazabat & Guéna [1], Erbil [2] and Larson [3], which show that tremendous experimental, analytical, and numerical studies have been conducted on droplet lifetime (evaporation rate), the internal flow inside droplet, the contact line dynamics, and the effects of substrate and liquid material, heating or no-heating of substrate, as well as the ambient temperature and humidity. Specifically, understanding affecting factors and their mechanisms on sessile droplet evaporation rate is extremely important, because it could not only provide a guide to optimize the lifetimes of evaporating droplets to achieve considerable efficiencies and economies in a variety of industrial contexts [4], but also deepen scientific understating of transportation phenomena during droplet evaporation.

Bexon [5] discovered two extremely different droplet behaviors (modes): (1) constant contact radius (CCR) mode, characterized by the reducing of contact angle and the pinning of contact line; (2) constant contact angle (CCA) mode, characterized by the receding of the contact line and the negligibly small variation of contact angle. They also pointed out in practice there were several stages of stick-slip behavior of contact line due to contact angle hysteresis caused by roughness and chemical in homogeneousness of substrate surface, which was later confirmed by Bourgès-Monnier & Shanahan [6]. It has been widely accepted now that a sessile droplet at first evaporates at CCR mode, and then switches to CCA mode with somewhat stick-slip dynamics of contact line, and finally changes to mixed mode characterized by simultaneous reducing contact angle and contact area, which was especially true on super-hydrophobic surfaces [7–9].

Almost all of the previous theoretical studies were based on two extreme approximations, i.e., quasi-steady state that assumes the time scale for the equilibrium of mass, momentum, and heat are much shorter than the droplet lifetime, and the diffusion-limited vapor transfer that supposes the vapor transport in the gas domain is attributed only by diffusion without the role of convection. Under further assumptions of isothermal droplet and spherical

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Nomenclature

c	molar concentration, mol/m^3
C_P	specific heat capacity, J/kg/ K
D	vapor diffusion coefficient in gas, m^2/s
$\boldsymbol{F}$	volumetric force, N
g	gravitational acceleration, m/s^2
H	relative humidity, 1
H_t	latent heat of vaporization, J/kg
k	thermal conductivity, W/(m·K)
$\dot{m}$	local evaporation flux, kg/(m^2 s)
M_a	molar mass of air, kg/mol
M_r	molar mass of liquid, kg/mol
$\boldsymbol{n}$	normal vector
p	pressure, Pa
r, z	cylindrical coordinates, m
r_c	curvature radius, m^{-1}
R	universal gas constant, J/mol/K
R_0	contact radius, m
t	time, s
T	temperature, K
$\boldsymbol{t}$	tangential vector of the interface
$\boldsymbol{u}$	velocity, m/s
V	volume of drop, μl
v_n	normal velocity, m/s

Greek symbols

α	thermal expansion coefficient, K^{-1}
μ	dynamic viscosity, Pa·s
ρ	density, kg/m^3
θ	contact angle, °
σ	surface tension, N/m
σ_T	surface tension's derivative with respect to temperature, N/m/K
$\boldsymbol{\tau}$	Stress tensor

Subscripts

∞	environmental condition
0	initial value
av	average
a, v	air and vapor
g, l, s	gas, liquid, solid phase
sat	saturated
surf	surface of droplet

shape, the diffusion equation in gas domain could be solved analytically to obtain analytical expressions for the relation of evaporation rate in terms of contact angle and contact radius, as given by Picknett & Bexon [5] and Popov [10]. With appropriate combination of CCR and CCA modes, the droplet lifetime could also be predicted as demonstrated by Stauber et al. [4]. Although these analytical results are very attractive because of their simplicity, their accuracies should always be checked from case to case by considering the validity of the isothermal and diffusion-limited assumptions.

Numerical simulation has become a more reliable tool for the prediction of evaporation rate owing to its capability to consider evaporative cooling as well as Marangoni flow simultaneously, both of which are deemed to have large effects on droplet evaporation [11]. In addition, numerical simulation could also provide more insight on the temperature and velocity fields, which are extremely important for understanding the mechanism of droplet evaporation but difficult to be investigated experimentally. However, numerical simulation of sessile droplet evaporation is not an easy task, mainly due to the transient nature of droplet evaporation with the continuous evolution of free surface. To avoid the tracing of free interface, which is in fact the most difficult part of numerical simulation of droplet evaporation, some previous numerical simulations [12] focused themselves on the steady-state evaporation at a certain contact angle and contact radius, i.e., at a certain instant of the whole droplet evaporation process. Although, some others [13–17] did simulate the transient variation of droplet volume (profile) with time, they actually decoupled the free interface evolution from the other transportation processes. The basic idea of the decoupling models is to convert the moving boundary problem of droplet evaporation to a time series of fixed boundary problems, and its basic steps are as follows: (1) the local evaporation flux at a certain time is evaluated by solving the steady-state heat, momentum and mass transfer equations, and then integrated over the liquid-gas interface to get evaporation rate (the mass loss per unit time); (2) this evaporation rate was then multiplied by an arbitrary time step to get the droplet volume reduction during the arbitrary time duration; (3) the new profile of spherical cap for the following time instant can then be described by assuming fixed contact line or fixed contact angle according to the new droplet volume.

Recently, the transient effect of heat and mass transfer on sessile droplet evaporation has been capturing more and more attentions. Lopes et al. [18] experimentally studied water droplets evaporation on silicon and glass substrates, which were decorated with a thin polystyrene layer to have the same surface wettability (contact angle). They also developed a numerical model describing the transient heat conduction in the substrate and in the droplet, and vapor diffusion in the gas phase, and solved it using a finite element method. Numerical simulation results were found to agree well with the experimental evaporation rate results, and reveal that the transient heat transport governs the evolution of local temperature distribution at the liquid–gas interface, and consequently the evaporation rate. Larson [3] pointed out in his review article that: (1) the quasi-steady state assumption for heat transfer is invalid for the low thermal conductivity substrate (especially when the thickness is large), because the thermal equilibration may take as long as the complete lifetime of the droplet evaporation; (2) even for substrate with high thermal diffusion coefficient, the early stage of evaporation could be highly transient because heat diffusion throughout the droplet will also take a certain time; (3) although the vapor concentration field near the droplet surface could quickly approach equilibrium state, the vapor field far from the droplet needs to take a much longer time to achieve quasi-steady state, and therefore some corrections on the boundary condition is necessary to get accurate result. Yang et al. [11] developed a fully transient sessile droplet evaporation model using Arbitrary Lagrangian-Eulerian (ALE) formulation, which takes into account the coupled transient transport processes in solid, liquid and gas phases as well as the continuous evolution of free surface. The numerical results revealed that: (1) the time to achieve quasi-steady state evaporation for a water droplet on glass depends greatly on the droplet initial contact angle: the larger the contact angle, the longer the time to achieve quasi-steady-state evaporation. This means that it takes time to transport heat through liquid water droplet as pointed out by Larson [3]; (2) the consideration of