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Thermal effects of substrate on Marangoni flow in droplet evaporation: Response surface and sensitivity analysis

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ABSTRACT

In this paper, the evaporation of sessile droplets resting on a substrate with different thermal properties is numerically investigated. Computations are based on a transient axisymmetric numerical model. Special attention is paid to evaluate thermal effects of substrate on the structure of bulk fluid flow in the course of evaporation. Numerical results reveal that Marangoni convection induced by non-uniform distribution of temperature along the interface exhibits three distinctly different behaviours: inward flow, multicellular flow and outward flow, consequently resulting in different particle depositions. It is highlighted that three factors (i.e. relative thermal conductivity, relative substrate thickness and relative substrate temperature) strongly affect the flow pattern. In order to further investigate the coupling effects of different influential factors, a Kriging-based response surface method is introduced. We model the flow behaviour as a function of continuous influential factors using a limited number of computations corresponding to discrete values of the inputs. The sensitivities of the Marangoni flow are also analysed using Sobol' index to study the coupling mechanisms of influential factors. The proposed method can be used to forecast the flow patterns for any input parameter without additional sophisticated computer simulation, and allows to confidently estimate an unknown environmental parameter.

1. Introduction

The evaporation of a liquid drop resting on a solid substrate is not only of fundamental scientific interest but also of great importance in a wide variety of industrial and scientific applications, such as evaporative self-assembly technique (DNA mapping, MEMS cooling) [1,2], evaporation-induced particle deposition (thin film coating, ink-jet printing) [3,4] and the design of more efficient heat transfer devices [5]. Among the mechanisms involved, the behaviour of Marangoni flow induced by temperature gradient along the liquid-gas interface can significantly influence deposition patterns upon drying. For this reason, understanding the flow characteristics inside the drop plays a vital role in controlling the distribution of the particle deposition in evaporating droplet.

Extensive theoretical and experimental researches have been motivated in recent years [6–8]. Most of the previous works were based on diffusion-limited process, normally focusing on predicting the evaporation rate. Hu & Larson [9] suggested a simple approximation to summarise the total mass flux across the droplet surface and then in turn to solve the free-surface problem. Other investigations like Ruiz & Black [10] provided insight into revealing the mechanisms within the liquid drop. Similarly, the experimental work by Girard et al. [11] explained that the flow inside the drop was induced by the non-uniform temperature distribution along the interface. Although surface-tension-driven flow (i.e. Marangoni flow) and resultant bulk flow have been extensively studied, the influence of thermal effects of the substrate on Marangoni flow patterns is less well-understood. Further theoretical analysis has pointed out that the direction of Marangoni flow is determined by both the relative thermal conductivity [12] and the relative substrate thickness [13], ultimately alters the deposition patterns. However, these investigations were limited to the case of non-heated substrate; the impact of substrate temperature was not taken into account. Furthermore, the above-mentioned studies were based on a pseudo-transient process which implies that the

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Nomenclature

r, z	cylindrical coordinates [m]
R	contact radius [m]
h_s	substrate thickness [m]
T	temperature [°C]
H	relative humidity
p	hydrodynamic pressure [N/m^2]
k	thermal conductivity [W/m K]
c_p	specific heat capacity [J/kg K]
D_0	diffusion coefficient [m^2/s]
K	mean curvature [m^{-1}]
c	molar concentration [kg/m^3]
u_Γ	normal velocity of the liquid-gas interface [m/s]
H_{vap}	latent heat of evaporation [J/kg]
j_m	local evaporation flux [kg/m^2 s]
J_m	overall evaporation flux [kg/s]
R_N	relative thermal resistance
CV_s	cross-validation value
S_{θ_i}	Sobol' index
f_{θ_i}	response surface for different contact angles

Greek symbols

θ	contact angle [°]
σ	surface tension [N/m]
σ_T	surface tension coefficient [N/m K]
ρ	density [kg/m^3]
μ	dynamical viscosity [Pa s]
α	thermal diffusivity [m^2/s]

Subscripts

0	initial or reference condition
∞	at the infinite in the gas region
l, s, g	liquid, solid, gas

Superscripts

$*$	dimensionless variable

Acronyms

LOO	Leave-One-Out
RE	Relative Error
RSM	Response Surface Method
SSA	Sobol Sensitivity Analysis

solution is a steady-state solution rather than a pure transient one. In this paper, we present numerical computations on the evaporation of sessile droplets resting on a heated substrate; we are particularly interested in evaluating thermal effects of the substrate on Marangoni flow in the course of evaporation, and determining typical bulk flow structures as a function of influential parameters related to the substrate. Indeed, based a transient, fully coupled three-phase (liquid-solid-gas) model, we clearly determined three distinct behaviours of Marangoni flow inside an evaporating droplet.

The efficient numerical technique is a more reliable tool for simulating the droplet evaporation process owing to its capability to consider the fully coupled mechanisms, like heat and mass transfer, thermal effects of substrate, evaporative cooling and thermocapillary convection [14,15]. In the present work, the effects of the substrate on Marangoni flow with respect to the influential parameters (thermal conductivity, thickness and substrate temperature) in a wide range are investigated. For this purpose, we need to simulate the evaporation process for all the possibilities of influential parameters. An alternative approach is to utilise response surface method (RSM). This approach aims to construct a continuous function of output by Kriging method [16,17], which allows to use the numerical results as a black-box with a limited number of inputs and outputs, and has proven to be a particularly effective tool for understanding fluid dynamics mechanisms and acoustic problems [18–22]. A leave-one-out (LOO) cross validation strategy [23] can be adopted to evaluate the reliability of the constructed response surface. Besides, the sensitivity analysis via Sobol' index [24,25] is able to quantify the relative importance of each input parameter in determining the response variability. By the Kriging-based response surface, the numerical results for any input model data can be rapidly forecast without further numerical computation. In terms of inverse problem, the Kriging-based response surface also helps to estimate the unknown input. It may happen in space experiments that some important input parameters, e.g. liquid concentration field in the vapour phase cannot be measured. In this case, the aforementioned unknown parameters can be estimated using the experimental results and the proposed response surface. The accuracy of parameter estimation strongly depends on the sensitivity of input parameters according to Sobol' sensitivity analysis (SSA). To the best of our knowledge, investigating the coupling mechanisms of multi-parameter on Marangoni flow by RSM and SSA, has not been reported in the literature.

The present paper aims to understand the behaviour of Marangoni flow in evaporating droplets and thus may be helpful to predict and control the deposition patterns in drying droplets. It is organised as follows. A transient axisymmetric numerical model for a sessile droplet evaporating on a heated substrate is developed in Section 2. Section 3 introduces a novel method based on RSM and SSA to evaluate the thermal effects of substrate on the structure of bulk flow induced by thermocapillarity. Results of single influential factor and the coupling mechanisms of multiple factors are presented and discussed in Section 4. Finally, the conclusions resulting from this investigation are summarised in Section 5.

2. Mathematical model

We consider a sessile drop with an initial contact angle θ_0 and a contact radius R_0 resting on a heated substrate of thickness h_s, as shown in Fig. 1. It is assumed that an axisymmetric sessile droplet

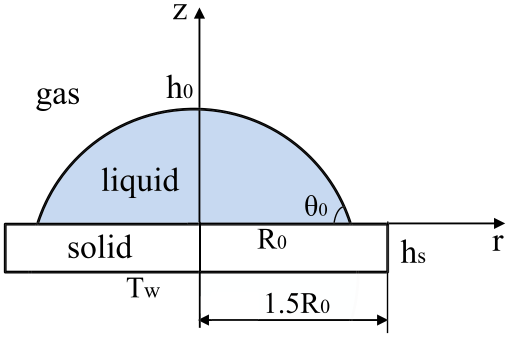

Fig. 1. A sessile drop resting on a heated substrate in a cylindrical coordinate system with radial coordinate r and axial coordinate z. The outer boundary of the computational domain is selected up to $50R_0$ of the surrounding air in order to eliminate the boundary effects and minimise the computational cost.