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Numerical investigation of the thermocapillary actuation behavior of a droplet in a microchannel

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ABSTRACT

The thermocapillary actuation behavior of a silicone droplet in a microchannel is numerically investigated in the present paper. The finite element method with the two-phase level set technique, which is ideally suitable for tracking the interfaces between two immiscible fluids, is employed to solve the Navier–Stokes equations coupled with the energy equation. The lower wall of the microchannel is subjected to a uniform temperature gradient, while the upper one is either adiabatic or isothermal. The thermocapillary flow inside the droplet is significantly affected by the thermal condition of the upper wall. When the upper wall is set to be adiabatic, a pair of asymmetric thermocapillary convection vortices initially occurs inside the droplet but these turn into a sole thermocapillary vortex once enough time has passed. For the isothermal case, a pair of asymmetric thermocapillary convection vortices always appears inside the droplet. The droplet initially accelerates for both the adiabatic and isothermal cases. The droplet velocity then decreases dramatically for the adiabatic case while it decreases slowly for the isothermal one. The dynamic contact angle of the droplet in a microchannel is strongly affected by the passage of the air flow over the droplet which is induced by the thermocapillary convection and the presence of the upper wall. The actuation velocity is enhanced by a higher temperature gradient, a reduction of microchannel height and a smaller contact angle for both adiabatic and isothermal cases.

1. Introduction

Recently, the liquid migration behavior in a microchannel has received wide attention because of potential applications in droplet-based microfluidics [1–3]. The migration velocity of a liquid droplet on a solid surface driven by thermocapillary actuation has been investigated in numerous studies [4–16]. The lubrication approximation [4–10] has been used to forecast the steady actuation velocity of the droplet. In this approach, the temperature field in the droplet is assumed to be dominated by conduction (small flow velocity) and the heat transfer to the surrounding air is negligible. Therefore, the temperature distribution along the free surface can be inferred from that imposed on the solid surface. Brochard [4] assumed the shape of the droplet to be approximately wedge-shaped with a small static contact angle (SCA). The movement of the droplet leads to variation in the contact angle, the so-called dynamic contact angle (DCA). The difference in the DCA between the advancing and receding sides is usually termed the contact angle hysteresis (CAH). The results indicated that the actuation velocity depends on the temperature gradient. Ford and Nadim [5] considered the shape of the droplet to be a two-dimensional, long, thin ridge pinned at a solid wall under the Navier slip condition. Their results indicated that the actuation velocity is strongly influenced by the slip length. Smith [6] studied the effect of the contact line motion on the apparent contact angle under the constant thermocapillary stress condition. His work showed that a thermocapillary convection cell would be generated inside the droplet by an imposed temperature gradient which would alter the free surface and the apparent contact angle. Chen et al. [7] based on the method developed by Ford and Nadim [5], computed the actuation velocity using the experimentally obtained height profile of a droplet, with a fixed CAH for different slip lengths. Gomba et al. [8] studied the thermocapillary migration of two-dimension droplets of partially wetting liquids on a non-uniform heated substrate. The shape of droplet varies with time instead of having a fixed shape. The droplet elongates into a long film profile when the contact angle is small, but becomes weakly distorted

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from its static shape for large contact angle. Large droplets may breakup into smaller ones. Their results also indicated that the advancing contact angle increases and the receding contact angle decreases as the thermal gradient increases. Pratap et al. [9] extended the lubrication approximation to take into account the three-dimensional axisymmetric spherical-cap shape of small drops. They also performed the experiments and observed that there was a significant decrease in the velocity of the contact line due to the evaporation. Karapetsas et al. [10] mentioned that the decrease in velocity of contact line is due to the change in the contact angle with temperature. The experimental results [11,12] showed that the final speed of the droplet increases with the footprint radius L and that the critical droplet size (below this size the droplet does not move) is roughly proportional to the inverse of the imposed temperature gradient. On the other hand, the experimental results of Pratap et al. [9] showed the critical droplet size to be independent of the imposed temperature gradient and insignificantly affected by the CAH. The experimental observations of Tseng et al. [12] indicated that the droplet shape would change during the actuation process. Nguyen and Chen [13–15] developed a numerical model to study the thermocapillary migration of a droplet on a horizontal solid surface in a large open air environment. In these works, the effect of heat transfer between the droplet and ambient was taken into account. Unlike the lubrication approach, the lowest temperature on the free surface always appears at or near the apex rather than at the contact line. Therefore, there are two asymmetric thermocapillary vortices inside the droplet which create the net momentum of the thermocapillary convection. This is the main driving-force for small droplet migration. Mondal et al. [16] investigated the effect of channel surface wettability and the inlet air velocity on the liquid droplet transport in microchannels.

For lab-on-a-chip (LOC) applications, the liquid droplet may be actuated in microchannels. Jiao et al. [17] studied the transient thermocapillary actuation of a liquid slug in a planar channel. The liquid slug can be manipulated anywhere in the channel using four integrated heaters and various heating strengths. Based on the results of Nguyen and Chen [13–15], it is known that as the liquid droplet is actuated in the microchannel through the imposed temperature gradient on the lower solid surface, the thermal condition at the upper solid surface may affect the actuation behavior of the droplet. On the other hand, the air motion induced by the thermocapillary convection may generate the pressure difference along the channel which will cause the imbalance of the droplet. This is a very important issue for manipulating the droplet within the microchannel. That has not been well studied.

In this study, the numerical simulation scheme developed by Nguyen and Chen [13–15] is utilized to investigate the thermocapillary actuation behavior of a small droplet in a microchannel. The droplet is placed at the lower wall of a microchannel which is subjected then to a uniform temperature gradient. The upper wall is either adiabatic or isothermal.

2. Physical model

A small liquid droplet is placed at the bottom solid wall in a microchannel with a cross-sectional area H × W in which H is the height and W is the length of the microchannel. The shape of the liquid droplet is initially assumed to be that of a cylindrical cap with a static contact angle θ, maximum height h_m, and footprint radius L (Fig. 1). A uniform temperature gradient G is imposed on the bottom wall, while the temperature of the top solid wall is either adiabatic or isothermal. Since the droplet is considered to be very small in size, the density of the liquid within it can be assumed to be constant and the influence from the body force can be neglected.

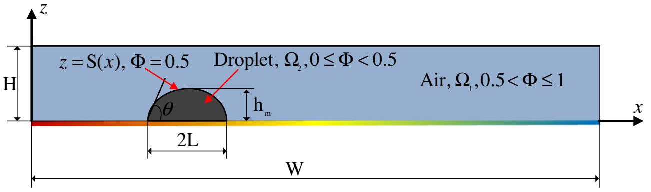

Fig. 1. Schematic representation used for computation. The value of the level set function Φ is equal to 0.5 at the air/droplet interface. The air phase (subdomain Ω_1) and the liquid phase (subdomain Ω_2) are represented by $0.5 < \Omega \leqslant 1$ and $0 \leqslant \Phi < 0.5$, respectively.

The two-dimensional equations for the conservation of mass, momentum, and energy for incompressible and Newtonian fluids are written as

$$\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial z}\right]_i = 0, \tag{1}$$

$$\rho_i\left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial z}\right]_i = -\frac{\partial p}{\partial x} + \mu_i\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2}\right]_i + F_x, \tag{2}$$

$$\rho_i\left[\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial z}\right]_i = -\frac{\partial p}{\partial z} + \mu_i\left[\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial z^2}\right]_i + F_z, \tag{3}$$

$$\rho_i \mathrm{C}_{\mathrm{P}i}\left[\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial z}\right]_i = k_i\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2}\right]_i, \tag{4}$$

where u_i and v_i are the velocity components in the x- and z- directions, respectively; p is the pressure and ρ_i is the fluid density; μ_i is the dynamic viscosity; $\mathrm{C}_{\mathrm{P}i}$ is the specific heat; k_i is the thermal conductivity; and T is the temperature. The subscripts i = "l" and i = "a" represent liquid and air, respectively. F_x and F_z are the surface tension force in the x- and z- directions, respectively.

The continuum surface force method developed by Brackbill et al. [18] is used to deal with the existence of the surface tension along the free interface. In this method, the surface tension is represented by a body force, which only acts on an infinitesimal thickness of the element at the free interface. The surface tension force at the free interface can be modeled by

$$F = \sigma\kappa\delta n, \tag{5}$$

where σ is the surface tension; δ is the Dirac delta function that is a nonzero value at the droplet/air interface only; n is the unit normal vector to the interface; and κ is the local interfacial curvature. The surface tension σ can be assumed to vary linearly with temperature [19]

$$\sigma = \sigma_{\mathrm{ref}} - \gamma_T(T - T_{\mathrm{ref}}), \tag{6}$$

where σ_{ref} is the surface tension at the reference temperature T_{ref} and $\gamma_T = -\partial\sigma/\partial T$ is the coefficient of the surface-tension.

The boundary conditions for the flow and temperature fields are given by

$$p = p_{\mathrm{a}};\ \frac{\partial u_a}{\partial x} = 0;\ \frac{\partial T_{\mathrm{a}}}{\partial x} = 0 \quad \text{at } x = 0 \text{ and } x = \mathrm{W}, \tag{7}$$

$$u_{\mathrm{a}} = v_{\mathrm{a}} = 0;\ \frac{\partial T_{\mathrm{a}}}{\partial z} = 0 \text{ or } T_{\mathrm{a}} = T_{\mathrm{ref}} \quad \text{at } 0 < x < \mathrm{W},\ z = \mathrm{H}, \tag{8}$$

$$u_{\mathrm{a}} = v_{\mathrm{a}} = 0 \quad \text{at } 0 < x < x_1 \text{ and } x_2 < x < \mathrm{W},\ z = 0, \tag{9}$$

$$T_i = T_{\mathrm{H}} - \mathrm{G} \times x \quad \text{at } 0 \leqslant x \leqslant \mathrm{W},\ z = 0, \tag{10}$$

where x_1 and x_2 are locations of the droplet's two contact points. The Navier slip condition is applied at the liquid–solid and gas–solid boundary