A combined computational and experimental investigation on evaporation of a sessile water droplet on a heated hydrophilic substrate

Manish Kumar, Rajneesh Bhardwaj

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Abstract
We numerically and experimentally investigate evaporation of a sessile droplet on a heated substrate. We develop a finite element (FE) model in two-dimensional axisymmetric coordinates to solve coupled transport of heat in the droplet and substrate, and of the mass of liquid vapor in surrounding ambient while assuming diffusion-limited and quasi-steady evaporation of the droplet. A two-way coupling is implemented using an iterative scheme and under-relaxation is used to ensure numerical stability. The FE model is validated against the published spatial profile of the evaporation mass flux and temperature of the liquid-gas interface. We discuss cases in which the two-way coupling is significantly accurate than the one-way coupling. In experiments, we visualized side view of an evaporating microliter water droplet using a high-speed camera at different substrate temperatures and recorded temperature of the liquid-gas interface from the top using an infrared camera. We examine the dependency of inversion of the temperature profile across the liquid-gas interface on the ratio of the substrate thickness to the wetted radius, the ratio of the thermal conductivity of the substrate to that of the droplet and contact angle. A regime map is plotted to demarcate the inversion of the temperature profile for a wide range of these variables. A comparison of measured evaporation mass rate with the computed values at different substrate temperature show that the evaporation mass rate increases non-linearly with respect to the substrate temperature, and FE model predicts these values close to the experimental data. Comparisons of time-averaged evaporation mass rate obtained by the previous and present models against the measurements suggest that the evaporative cooling at the interface and variation of diffusion coefficient with the temperature should be taken into account in the model in order to accurately capture the measurements. We compare the measurements of time-varying droplet dimensions and of temperature profile across the liquid-gas interface with the numerical results and found good agreements. We quantify increase in the evaporation mass flux and evaporation mass rate by the substrate heating and present the combined effect of substrate heating, the ratio of the substrate thickness to the wetted radius, substrate-droplet thermal conductivity ratio and the contact angle on the evaporation mass rate.

1. Introduction
In the last decade, evaporation of a sessile, pure liquid droplet on a solid surface is a much-studied problem, owing to several technical applications such as evaporative spray cooling and inkjet printing, etc. The physics involved during the evaporation is briefly described as follows. In the absence of any external convection, the evaporation occurs by diffusion of liquid vapor in surrounding gas. The evaporation mass flux (\( j \)) [kg/m\(^2\) s] on the liquid-gas interface is non-uniform, and the largest evaporation near the contact line generates evaporative-driven radially outward flow inside the droplet [1]. Heat transfer occurs mostly by conduction in the droplet and substrate and the non-uniform evaporation rate also results in non-uniform cooling at the liquid-gas interface by latent heat of evaporation. Depending upon the roughness of the substrate, the contact line may remain pinned or may recede at a constant contact angle during the evaporation.

analytically solved the vapor concentration field using toroidal coordinates and gave expressions of evaporation mass flux, evaporation rate and evaporation time, valid for any arbitrary contact angle. The sign of temperature gradient along the liquid-gas interface determines the direction of thermocapillary (or Marangoni) flow inside the droplet and is influenced by contact angle [5], the ratio of thermal conductivity of the substrate to that of droplet [6] and the ratio of substrate thickness to wetted radius [7].

In the context of theoretical studies for heated substrates, Sobac and Brutin [8] modeled the droplet evaporation by extending the model of Hu and Larson and by considering the temperature of the liquid-gas interface equal to substrate temperature, thereby ignoring the heat transfer in droplet and substrate. In this study [8], comparisons of the model predictions with measurements showed that the heat transfer should be considered in the model for larger substrate heating, in order to accurately capture the measurements. Zhang et al. [9] solved energy equation in the droplet and substrate in axisymmetric coordinates assuming quasi-steady evaporation. They used spatial profile of evaporation mass flux described by Hu and Larson [2] in their model and showed that the spatial profile of temperature at the liquid-gas interface depends on the ratio of thermal conductivity of the substrate to that of the droplet. Simulations by Barmi and Meinhart [10] quantified the internal convection against Marangoni number and they found that the Marangoni convection becomes negligible as the droplet volume decreases during the evaporation. Maatar et al. [11] numerically investigated the evaporation of water and volatile liquid droplets considering transient effects while modeling the energy equation in the droplet and the substrate. They showed that the transient effects are important to consider in the model for a thicker substrate with lower thermal diffusivity. Xu and Ma [12] proposed a “combined field approach” to couple the energy equation and Laplace equation of diffusion of vapor concentration. By assuming a linear variation of saturated concentration with temperature, they proposed a unified way to solve the two governing equations. This method does not need iterations between the two governing equations. In a follow-up paper, Wang et al. [13] extended the model of Xu and Ma [12] to investigate the combined effect of evaporative cooling, and thickness and thermal conductivity of the substrate. They showed that for larger evaporative cooling, the influence of substrate is significant. Liu et al. [14] numerically showed that the transient effects during the evaporation of volatile droplets are important and assumption of quasi-steady evaporation is not valid in such cases. Very recently, Buchenna et al. [15] proposed a model to study the flow inside the evaporating water droplet on a heated substrate and showed the existence of multicellular flow pattern at smaller contact angles and larger substrate heating.

In the context of recent experimental studies, David et al. [16] experimentally investigated the effect of substrate thermal conductivity and concluded that it influences the evaporation mass rate. In particular, significant evaporating cooling can occur by an insulating substrate. Bhardwaj et al. [17] recorded impact and evaporation of an isopropanol droplet using high-speed visualization. They used a laser-based thermo-reflectance method to measure liquid-solid interface temperature and showed that the temperature increases exponentially during the impact and it undergoes a slight linear decrease during the evaporation. Ghasemi and Ward [18] experimentally showed that the thermocapillary convection is the dominant mode of heat transfer near the contact line, however, heat conduction dominates at the apex of the droplet. Sobac and Brutin [8] experimentally investigated the thermal effects of the substrate by recording an evaporating water droplet on hydrophilic and hydrophobic engineered aluminum substrates. Lopes et al. [19] investigated the effect of thermal properties of the substrate on evaporation time of a sessile droplet and found that evaporation accelerates on a substrate with larger thermal conductivity. Very recently, Bazargan and Stoebel [20] experimentally investigated the effect of substrate conductivity on evaporation of water droplets of 100–500 μm diameter. The comparison of these measurements with a one-dimensional heat transfer model showed the existence of a critical radius of sessile droplet below which substrate cooling effects the total evaporation time.

Several recent studies have reported the measurement of liquid-gas interface temperature using infrared thermography. Brutin et al. [21] visualized thermal-convective instabilities during evaporation of droplets of volatile liquids on a heated surface using infrared visualization. Fabien et al. [22] recorded temperature of the liquid-gas interface of an evaporating water droplet on heated substrates using infrared thermography and plotted the temporal evolution of the temperature in different cases of substrate temperatures. Very recently, Fukatani et al. [23] recorded hydrothermal waves in an evaporating ethanol droplet using infrared thermography and showed that these waves can be influenced by relative humidity.

Most of the previous models of the evaporating sessile droplet on non-heated or heated substrates were based on the following assumptions: heat transfer is only in the axial direction [7], liquid-gas interface temperature is equal to substrate temperature [8] and saturated liquid-vapor concentration varies linearly with temperature [12,13]. The expressions of evaporation mass rate and spatial variation of evaporative flux reported in previous studies [2,4] are valid for a substrate at ambient temperature. In addition, the combined effect of parameters, namely, substrate heating, substrate thickness, contact angle, thermal properties of droplet and substrate, substrate heating have not been reported before. To this end, we present a combined numerical and experimental study with the following objectives. First, we develop and validate a model for the droplet evaporation on a heated substrate which solves coupled energy and mass transport equation in order to account for heat transfer in the droplet as well substrate. Second, using the model, we investigate the effect of geometry and thermophysical properties of the droplet and substrate, and substrate temperature on evaporation characteristics. Third, we perform experiments to measure time-varying droplet shapes using high-speed visualization and temperature of the liquid-gas interface using infrared thermography. Finally, the measurements are compared with the model predictions in order to investigate the fidelity of the model and understand the coupled physics.

2. Computational model

We extend the models reported in previous studies [2,8,12,13] to account the evaporation of a sessile droplet on a heated hydrophilic substrate. In particular, we develop a two-way coupling of the energy equation in droplet and substrate and transport of liquid vapor outside the droplet. The definitions of the notations used in the following sections are listed in Table 1.

2.1. Governing equations and boundary conditions

We consider diffusion-limited, quasi-steady evaporation of a sessile droplet with a pinned contact line on a heated hydrophilic substrate. The wetted diameter of the droplet is taken lesser than capillary length so that the droplet maintains a spherical cap shape throughout the evaporation. The validity of the quasi-steady evaporation is examined by considering the ratio of heat equilibrium time in a droplet (t_h) and its total evaporation time (t_f), as discussed by Larson [24] and is given by,

\[ \frac{t_f}{t_h} \approx \frac{1}{5} \frac{D}{\varepsilon c_{\text{sat}}} \frac{\left( \frac{R}{L} \right)^2}{\rho_g} \]

(1)
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