Fluid flow inside and outside an evaporating sessile drop

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Abstract. The sessile drop evaporation is a phenomena which is extensively studied in the literature, but the governing effects are far from being well understood especially those involving movements taking place in both liquid and gas phases. The present work numerically studies the flow within and around an evaporating sessile drop. The flow is induced by the strong mass loss at contact line, the thermo-capillary effect and the buoyancy effect in the surrounding air. The results showed that buoyancy-induced flow in gas phase weakly influences thermo-capillarity-induced flow in the liquid phase. Buoyancy effect can strongly modify the temperature distribution at liquid-gas interface and thus the overall evaporation rate of the drop when the substrate is heated.

1. Introduction

Sessile drop evaporation is a process, which has extensive applications in biochemical assays, thin film coating, spray cooling, microelectronics, nano-devices and others. It is a complex physical problem which involves fluid flow, heat and mass transfer as well as interactions between the solid substrate, the liquid droplet and the surrounding gas throughout moving interfaces and a pinned or receding contact line [1]. Recently Larson [2] summarized analytical, numerical and experimental literature works on drying sessile droplets and deposition of suspended materials. He presented a list of useful dimensionless groups governing mass, momentum, and heat transfer effects in the droplet, the surrounding gas and the substrate.

One of the most important applications of the sessile drop evaporation in thin film technology is the final pattern of the solid particles deposits on substrates. The particle deposition is strongly affected by the flow inside the drop. The competition of the flow induced by the privileged evaporation near the contact line, the thermo-capillarity and the buoyancy effects, is strong during drop evaporation, and the prevalence of one or two effects rules the flow direction inside the drop. Several works were conducted to study the influencing parameters, which define flow patterns in the evaporating sessile drops [3-22].

The present work is a numerical study of the convective internal and external flow of an evaporating water sessile drop. Few previous studies assumed that the surrounding air is in movement [13]. Nevertheless, understanding dynamics of both liquid and gas allows to better analyzing the evaporation kinetic of the drop and handling and controlling the strains of particle deposits after drying on substrates of different natures and in heated or non-heated cases. In this framework, a numerical model is developed by taking into account (1) the flow induced by the strong liquid loss...
near the contact line, (2) the thermo-capillary flow resulting from the surface tension gradient due to temperature variation at the drop surface, and (3) the flow induced by the buoyancy in the surrounding air. The objective is to analyze the internal and external flow intensity and the flow pattern resulting from the competition of the driving effects as well as its impact on the evaporation rate.

2. Mathematical model
We consider a small water drop on a substrate of high thermal conductivity. The surrounding air is at ambient temperature $T_w = 25°C$ and relative humidity $Ha = 40\%$. The lower face of the substrate is maintained at a temperature $T_w = T_x$. The drop evaporation is assumed to occur with pinned contact line. Buoyancy effect is included in the model by using the Boussinesq approximation. The proposed mathematical model is the same as in our previous works [21, 22], except in gas phase where the momentum equations are added to take into account the flow in the surrounding gas and then the convective term is added to energy and concentration equations. Convective flow in both liquid and gas phases is governed by the conservation equations of mass, momentum and energy coupled with vapor transport equation in the surrounding air and heat conduction equation in the substrate. Mass and momentum conservation and energy balance at the liquid-gas interface are expressed in dimensionless forms as follows:

i) Mass conservation,

\[
\left(\vec{\dot{W}}_l - \vec{\dot{W}}_i\right) \cdot \tilde{n} = \frac{R_{\rho g}}{Le Ma} \left(\frac{\Delta C}{\rho_l}\right) \vec{J}^* \cdot \tilde{n} \tag{1}
\]

where $\tilde{n}$ is a normal unit vector, $\vec{\dot{W}}_l$ is the velocity of the moving interface, $\vec{\dot{W}}_i$ is the velocity of a liquid (gas) particle, $\vec{J}^*$ is the liquid density and $\Delta C$ is equal to $(C_v(T_w) - Ha C_v(T_x))$ where $C_v(T)$ is the saturated vapor concentration. Different dimensionless numbers appear in Eq. (1): Marangoni number ($Ma$), Lewis number ($Le$), ratio of gas/liquid density ($R_{\rho g}$), ratio of gas/liquid thermal diffusivity ($R_{\alpha g}$).

ii) Shear-stress balance,

\[
\left(\vec{\tilde{n}} \tilde{\tau}\right) - \left(\vec{\tilde{n}} \tilde{\tau}_g\right) \cdot \vec{\tilde{t}} = \tilde{\nabla} T^* \cdot \vec{\tilde{t}} \tag{2}
\]

where $\vec{\tilde{n}}$ is a tangential unit vector and $\tilde{\tau}$ is the dimensionless stress tensor. The temperature gradient ($\tilde{\nabla} T^*$) in Eq. (2) represents the term of thermo-capillary effect.

iii) Energy balance,

\[
\frac{Ja}{Le}\left(\frac{\Delta C}{\rho_l}\right) \vec{J}^* + \left(R_{\rho g} T^* - \nabla T^*\right) \cdot \tilde{n} = 0 \tag{3}
\]

where $R_{\rho g} = k_{\rho g} / k_l$ is the ratio of gas/liquid thermal conductivity, $Ja = h_{lg} / (c_{pl} \Delta T)$ is the Jacob number, $\Delta T$ is equal to $(T_w - T_x)$, $h_{lg}$ is the latent heat of vaporization and $c_{pl}$ is the liquid specific heat. The quasi-steady state governing equations with associated boundary and interface conditions are solved numerically. The concentration gradients at the drop surface are then used to evaluate the evaporation rate and deduce the drop lifetime.

3. Numerical procedure
Finite volume method and staggered grid are applied to resolve the mathematical model [23]. Coupling of velocity and pressure fields in fluid phases is addressed by the SIMPLE algorithm. Power law differencing scheme (PLDS) is used to consider the contribution of convection and diffusion in the transport phenomena. The algebraic equations resulting from the finite volume discretization are solved by a combination of the tridiagonal matrix algorithm (TDMA) and the Gauss-Seidel iterative method along with under-relaxation. Solutions of velocity, temperature and concentration fields reach satisfactory convergence during the iterative process once the maximum relative error on the
dependent variable (u, v, T, C) is smaller than 0.1%. The maximum allowable absolute residue in the mass conservation equation is less than $10^{-10}$ and less than $10^{-5}$ in other conservation equations.

The elaborated computational program is validated with previous works in the literature. Hereafter is presented the comparison of our results with those of the numerical study of Yang et al. [1]. Figure 1 shows flow field in both liquid and gas phases for an evaporating sessile drop at a contact angle of 50°. There is a good agreement between the compared results.

![Figure 1](image)

**Figure 1.** Comparison with numerical results of velocity fields obtained by Yang et al. (water sessile droplet with $\theta=50^\circ$ and $R=0.95$ mm, glass substrate with $k_g=0.96$ W/mK and $e_w=0.2$ mm, $T_w=50^\circ$C, $T_a=22^\circ$C and $Ha=50\%$).

### 4. Results and discussion

Results are presented for a water drop of 10 mm$^3$ initial volume deposited on a substrate with high thermal conductivity. Velocity and temperature fields are plotted in Fig. 2 for a contact angle $\theta = 20^\circ$ and wall temperature $T_w=50^\circ$C. A tri-cellular flow appears in the drop due to the thermo-capillary effect in heating conditions and confined geometry of the drop at $\theta = 20^\circ$. The external flow near the drop surface is driven by the internal flow through thermo-capillary effect, whether the buoyancy in the gas is included or not. This is due to the viscosity of the liquid which is much greater than that of the gas. The intensity of fluid flow in gas phase increases with buoyancy effect consideration, and this can affect the temperature distribution also in gas phase. This figure indicates that taking into account the buoyancy effect weakly influences fluid flow and temperature distribution in liquid phase.

![Figure 2](image)

**Figure 2.** Velocity and temperature fields for a contact angle $\theta=20^\circ$ and wall temperature $T_w=50^\circ$C.
In Fig. 3, the temperature distribution at drop surface is presented for different models: diffusion model, model taking into account only fluid flow in liquid phase, model taking into account fluid flow in both liquid and gas phases without buoyancy effect, and finally a complete model which takes into account fluid flow in the two phases with buoyancy in surrounding gas. It is clearly shown that the buoyancy in the air can increase the importance of the thermos-capillarity especially under the heating conditions and thus influence the internal flow even if this is weak. The buoyancy effect decreases temperature at drop surface. This is due to the gas movement which takes the water vapour far from the drop and as result the evaporation mass flux increases as well as heat transfer from drop surface to surrounding air. At the opposite, the internal flow rather implies an increase in the surface temperature at the edge of the drop by comparison with the diffusion model, although globally the evaporation rate also increases due to thermal convective effects in the liquid phase.

![Figure 3](image.png)

**Figure 3.** Temperature profile at drop surface for $q = 20^\circ$ and $T_w = 25$ or $50^\circ$C.

Finally, we finish this study by analysing the effect of fluids flow on the evaporation kinetics. The evolution in time of the evaporation rate is of great interest, because of its applications in cooling, painting, coating and others. In several numerical works, the authors were interested on evaporation rate evolution but with models not considering flow in the gas phase. In the figure bellow (Figure 4), we present the evolution in time of the evaporation rate density (evaporation rate per drop surface) in both heated and non-heated cases. The results of two different models are given. In the first model, the flow in liquid and gas phases is taken into account, but without considering the buoyancy effect. In the second model, all effects are considered as well as buoyancy convection in the gas phase. Results show that the buoyancy convection has a significant effect on evaporation rate density especially when the substrate is heated. The effect of drop surface variation on decreasing the evaporation rate is more important than that of liquid or gas flow on its increase.

![Figure 4](image.png)

**Figure 4.** Evolution of the evaporation rate density during sessile drop evaporation on a substrate of high thermal conductivity. The substrate is heated ($T_w = 50^\circ$C) or non-heated ($T_w = 25^\circ$C).
5. Conclusions

The results presented in this work showed that, when the fluid flow is considered inside and outside an evaporating sessile drop, the governing effect is the thermo-capillarity; it mainly imposes the direction in both liquid and gas phases. The comparison between results obtained with the model taking into account buoyancy in gas phase, and those obtained with the model neglecting it, showed that the effect of buoyancy convection in the gas on liquid flow intensity and direction is negligible, but its effect on temperature distribution at liquid-gas interface is important. The evaporation rate is underestimated by the model without buoyancy effect in the gas phase, especially in heated substrate cases. From these results we can conclude that the complete and appropriate model to better estimate, fluid flow, temperature distribution, and evaporation rate, is the model taking into account fluid flow inside and outside the evaporating sessile drop.

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