Effect of substrate thickness and thermal conductivity on an evaporating sessile drop

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Abstract. A quasi-steady state diffusion model is developed to predict the evaporation of a sessile drop of water and analyze the effect of substrate properties. A numerical approach based on the finite volume method is implemented to assess the heat and mass exchanges at the drop surface. Numerical results illustrate the effect of the thermal conductivity and the thickness of the substrate on the temperature and concentration fields. It is evidenced that a decrease in thermal conductivity of the substrate or an increase of its thickness has a similar cooling effect on the drop and widen the extent of the cold zone resulting from the evaporation. The influence of these two parameters is kept constant all along the evaporation process for a pinned drop.

1. Introduction
Evaporation phenomenon is encountered in several engineering and industrial processes such as drying, welding, cooling, combustion, nuclear engineering and microelectronics. A sessile drop is a drop which is deposited on a solid substrate where the wetted area is limited by a contact line and characterized by contact angle, contact radius and drop height. Understanding the physics of evaporation of a sessile drop requires a detailed analysis of heat and mass transfer at various interfaces: liquid-gas, solid-gas and solid-liquid. Many authors investigated this problem in order to study the effect of the wettability [1], the effect of the thermal properties of substrate [2, 3], the Marangoni effect or the effect of surrounding gas [4, 5]. Recently Erbil [6] presented an exhaustive review of the related published works. He discussed the basic theory comprising evaporation of micrometer and millimeter sized spherical drops, self cooling on the drop surface and evaporation rate of sessile drops on solids. Numerical models were also developed by Ait saada et al. [7] who used a convection-diffusion model to analyze the effect of buoyant convection in the surrounding air on heat and mass transfer phenomena during the evaporation of a pinned water sessile drop. They concluded that the diffusion model underestimates the evaporation rate in comparison to that obtained with a convection-diffusion model.

In this study, a numerical analysis is carried out using a diffusion model to work out the problem of evaporation of a small water drop on a horizontal solid substrate. The substrate of different thicknesses
can be a perfect thermal insulator \((k_s \approx 0)\), a perfect heat conductor \((k_s \to \infty)\) or having intermediate thermal conductivities \(k_s\). The model proposed accounts for heat conduction in solid, liquid and gas phases and for water vapor diffusion in the surrounding air. The computer program is implemented to couple between the substrate, the drop and the surrounding air. The temperature and concentration profiles are first determined and then the local heat flux is computed at the liquid-gas interface. The mass transfer is quantified locally by the mass flux and globally by the evaporation rate on the drop surface. The effect of relevant parameters such as thickness and thermal conductivity of the solid substrate are discussed.

2. Mathematical Formulation
A pure water drop of 10 mm\(^3\) and 78° initial volume and contact angle, respectively, is deposited on a non-heating horizontal substrate of thickness \(e_w\) and thermal conductivity \(k_s\), as shown in figure 1. The substrate has the shape of a disc with a very large radius and it is thermally insulated on the lateral wall. The drop evaporation occurs in a surrounding moist air at ambient temperature \(T_\infty\) of 25°C and relative humidity \(H_\infty\) of 40%. The drop has a shape of a spherical cap controlled by the surface tension effects because its size is selected lower than the capillary length \(l = (\sigma / \rho \cdot g)^{1/2}\) (equal to 2.69 mm for water), where \(g\) is the gravitational acceleration, \(\rho\) is the liquid density and \(\sigma\) is the surface tension. Three modes of evaporation are usually reported in the literature, namely the constant contact radius mode (pinned drop), the constant contact angle mode (de-pinned drop) and the stick-slip mode which combines the two previous modes [1]. During the evaporation, the drop is assumed pinned, its wetting radius \(R\) is kept constant and the contact angle \(\theta\) varies with time.

![Figure 1. Water drop of spherical cap shape deposited on a horizontal substrate.](image-url)
Mass transfer in the surrounding gas as well as heat transfer in the three phases are supposed to evolve symmetrically around the vertical axis (oz) and in quasi steady state regime due to the slow evaporation process inducing a slow motion of the liquid–gas interface. The mathematical formulation of the considered physical problem is based on the concentration equation in the gas phase and on the conservative energy equation in the gas, liquid and solid phases. The computational domain is constituted with three zones: zone (I) is the substrate, zone (II) is a hemisphere encompassing the drop and its close surrounding air and zone (III) is the remaining gas phase. The governing equations are written in toroidal coordinates ($\alpha, \beta$) in zone II, in cylindrical coordinates (r, z) in zone I and in spherical coordinates ($r', \phi$) in zone (III). The toroidal coordinate system allows better handling and localizing the moving liquid-air interface ($\beta=\beta_i$).

Boundary conditions associated with the governing equations are indicated in figure 1. No temperature jump condition and continuity condition of heat and mass flux at the interface between zones (II) and (III) are applied. The same conditions are also imposed on the upper face of the substrate in addition to an impermeable wall condition with respect to mass transfer. These interface conditions are expressed in dimensionless form by:

i) interface between zones (II) and (III),

$$T^*_g = T^*_{gIII}, \quad \left( \frac{\partial T^*_g}{\partial r^*} \right)_\beta = -\left( \frac{\partial T^*_{gIII}}{\partial r^*} \right)_I \quad \text{and} \quad \left( \frac{\partial C^*_g}{\partial r^*} \right)_\beta = -\left( \frac{\partial C^*_{gIII}}{\partial r^*} \right)_I \quad (1a)$$

ii) interface between solid and liquid phases,

$$T^*_s = T^*_l \quad \text{and} \quad Rk_s \left( \frac{\partial T^*_s}{\partial z^*} \right)_0 = -\left( \frac{\partial T^*_l}{\partial z^*} \right)_\pi \quad (1b)$$

iii) interface between solid and gas phases,

$$T^*_s = T^*_g, \quad Rk_g \left( \frac{\partial T^*_g}{\partial z^*} \right)_0 = Rk_g \left( \frac{\partial T^*_s}{\partial r^* \partial \phi} \right)_0 \quad \text{and} \quad \left( \frac{\partial C^*_g}{\partial z^*} \right)_0 = 0 \quad (1c)$$

$Rk_s$ and $Rk_g$ are solid/liquid and gas/liquid thermal conductivity ratio, respectively. The variables are scaled in the dimensionless form of governing equations, boundary and interface conditions with respect to the length $R$, the reference temperature $T_\infty$ and the concentration difference $\Delta C = (1 - H_\alpha) C_s (T_\infty)$ where $C_s(T_\infty)$ being the saturation concentration at $T_\infty$. The dimensionless temperature and concentration are given by $T^* = (T - T_\infty) / T_\infty$ and $C^* = (C - C_\infty) / \Delta C$, respectively, where $C_\infty = H_\alpha C_s (T_\infty)$. The dimensionless metric coefficients of the toroidal coordinate system are noted: $H = H_\alpha = H_\beta$ and $H_\phi$ where $\phi$ is the third coordinate.

In addition, no temperature jump condition is applied at the surface of the drop where air is in a saturated state; its vapor concentration depends on temperature according to a polynomial relationship:

$$C_v(T) = \sum_{i=0}^{4} a_i T^i \quad (2a)$$
The coefficients $a_0, a_1, a_2, a_3$ and $a_4$ are chosen to fit experimental data of Raznjevic [8]. Moreover, the dimensionless mass flux of evaporation from the drop, noted $J^*$, must satisfy the local energy balance, expressed by:

$$
\left( \frac{\Delta C}{\rho_g} \right) J^* = \frac{R_k}{Le} \left( \frac{\partial T_c^*}{Hc\beta_i} \right) \bigg|_{\beta_i} + \frac{\partial T_c^*}{Hc\beta_i} \bigg|_{\beta_i} = 0 \quad (2\ b)
$$

$Ja = h_{tg} / (c_{pg} T_c)$ is the Jacob number where $h_{tg}$ is the latent heat of evaporation and $c_{pg}$ is the gas specific heat. $Le = (\alpha_T / D)_g$ is the Lewis number where $D$ is the vapor diffusion coefficient in gas and $\alpha_{tg}$ is the gas thermal diffusivity.

The local mass transfer on the drop surface is evaluated by the evaporation flux $J$ which is related to the concentration gradient. In a dimensionless form, it is expressed as:

$$
J^* = \frac{J}{D \frac{\Delta C}{R}} = \frac{\partial C^*}{Hc\beta_i} \bigg|_{\beta_i} \quad (3\ a)
$$

The evaporation rate $M^*$ over the whole drop surface is determined by the following equation:

$$
M^* = \frac{M}{2 \pi R D \Delta C} = \int_0^\pi \frac{\partial C^*}{Hc\beta_i} \bigg|_{\beta_i} H_d Hda \quad (3\ b)
$$

3. Numerical procedure

The set of governing partial differential equations with the corresponding boundary and interface conditions are solved by means of the control volume method [9]. A zonal grid is applied in the computation domain in corresponding coordinate system in each zone and taking care of ensuring conservation of heat and mass fluxes at interfaces. A grid sensitivity analysis is carried out in order to choose the adequate number of nodes to simulate accurately the evaporation of a sessile drop. A 116×104 grid in the zone (II) showed to be enough for acceptable accuracy. A finer grid of 221×203 nodes yields results with a maximum relative difference of 0.02% at the expense of higher computation time. The node spacing in zone (II) is of 15.6 µm; it is even smaller near the interfaces (1.56 µm) and 0.156 µm very close to the contact line. A second order central differencing scheme (CDS) is used to discretize the diffusion equation. The set of obtained algebraic equations are solved using a combination of the tridiagonal matrix algorithm TDMA and the Gauss-Seidel iterative method. The temperature and concentration solution reach satisfactory convergence during the iterative process once the maximum relative error on the dependent variable ($T^*, C^*$) is lower than 0.1% and the maximum allowable absolute residue in the conservative equations is less than $10^{-5}$.

The computer program is validated by comparing simulation results with published results in the literature. Figure 2 shows that the used diffusion model fits with an excellent agreement the experimental data of Hu and Larson [10] and Song et al. [11] for the evolution of the water drop volume during evaporation on a glass slide. A deviation of less than 5% from the experimental results is obtained when the glass slide is considered as an isothermal surface at room temperature of $25^\circ$ C.
The present work aims to study the effect of thermal conductivity and the effect of the substrate thickness. We consider a water drop of 10 mm³ placed on a substrate covered by a very thin layer of aluminum imposing an initial contact angle of 78°.

Temperature and concentration fields are shown in Figure 3 for θ = 78° corresponding to the beginning of evaporation. Two substrates are considered: a perfect insulator (k_s ≈ 0) and a perfectly heat-conducting material (k_s → ∞). The isotherms distribution exhibits closed contour curves in the region of the liquid-gas interface corresponding to a cooled zone resulting from the phase change accompanied by a decrease in temperature below 25°C. So there is a cooling effect in the drop and in the vicinity of this one both in the substrate and in the surrounding air. For k_s ≈ 0, the temperature is highly variable in the substrate and the environment gas while it is almost constant in the droplet. In this case the needed energy for evaporation comes only from the surrounding air. The saturation concentration is constant and the water vapor diffuses almost uniformly to the atmosphere along the drop surface due to the shape of the drop close to a hemisphere (θ = 78°). The increase in thermal conductivity of the substrate yields an increase in temperature in the three phases, resulting in a reduction of the extent of the cold zone. The minimum temperature located at the top of the drop is raised and temperature gradients in the liquid phase increase while they decrease in the other two phases. Concentration gradients are high close to the liquid-gas interface and take the highest value at the contact line where most of the evaporation occurs.

![Figure 2](image-url)  
*Figure 2. Drop volume variation with time predicted using the developed numerical simulation. The results are compared with experimental results of Hu and Larson (V₀ = 0.54 mm³, θ₀ = 42°, D = 26.1×10⁻⁶ m²/s, Hₐ = 40%) and Song et al. (V₀ = 3.64 mm³, θ₀ = 57.2°, D = 25×10⁻⁶ m²/s, Hₐ = 40%).*

![Figure 3](image-url)  
*Figure 3. Effect of substrate thermal conductivity on isotherms and iso-concentrations distribution for θ = 78°: (a) kₜ ≈ 0 (b) kₜ → ∞.*
The effect of the substrate thickness is illustrated through temperature and concentration plots of Fig.4. An increase of the thickness has a similar effect as a decrease of the thermal conductivity because these two parameters are involved in the thermal resistance of the substrate. Thickening of the substrate causes a wider cold zone and a greater cooling of the drop. The temperature gradient is reduced at the solid-liquid interface and it is augmented at the liquid-gas interface. In terms of concentration gradient, it decreases at the drop surface and it yields less evaporation because less thermal energy comes from the substrate and most of heat arrives from the surrounding air. A thick or extremely thick substrate (\(e_w \geq 10\) mm) is considered as a semi-infinite medium that continues to thermally feed the drop in an asymptotic way.

Figure 4. Effect of substrate thickness on isotherms and iso-concentrations distribution for \(\theta = 78^\circ\) and \(k_s = 0.025\) W/mK: (a) \(T_{\text{min}} = 22.29, C_{\text{max}} = 0.0205\) (b) \(T_{\text{min}} = 19.43, C_{\text{max}} = 0.0167\) (c) \(T_{\text{min}} = 17.56, C_{\text{max}} = 0.0150\) (\(\Delta T = 0.25^\circ\text{C}, \Delta C = 0.0005\) \(\mu g/mm^3\)).

Figure 5 shows the distribution of evaporation mass flux (J) on the drop surface. This flux increases when the liquid-gas interface locally receives more heat from the liquid phase because of the increase in the thermal conductivity of the substrate. It is uniformly distributed along the drop surface except near the contact line where the evaporation flux is higher. For a perfectly conducting substrate, J starts increasing from a certain distance to the contact line and then it is substantially augmented at the contact line. As the thermal conductivity of the substrate diminishes the evaporation flux increases in a less pronounced manner at the contact line and in the limiting case of \(k_s = 0\), J is almost uniformly distributed along the liquid-gas interface. This result is found at a high value of contact angle of 78°.
At smaller values of contact angle the effect of $k_s$ on the evaporation flux is reduced and vanishes completely at very small value of $\theta$.

![Graph](image)

**Figure 5.** Effect of substrate thermal conductivity on the local evaporation flux on the drop surface for $\theta = 78^\circ$.

In terms of overall mass transfer, Figure 6 shows the variation of the evaporation rate versus the contact angle for several values of the thermal conductivity of the substrate. It is depicted that the evaporation rate can vary between two limits. The upper limit corresponds to the case $k_s \to \infty$. In this case, the saturation concentration at the drop surface which strongly depends on temperature is highly influenced by heat coming from the liquid phase. The lower limit represents the idealized adiabatic substrate with $k_s = 0$ in which case heat arrives at the drop surface only from the surrounding air. The evaporation rate is shown to vary slightly with contact angle.

![Graph](image)

**Figure 6.** Evaporation rate versus contact angle for various substrate thermal conductivities.

To summarize the effect of the two studied parameters i.e. substrate thermal conductivity and its thickness, we plot in Fig.7 the evaporation rate versus $e_w$ and $k_s$ for two values of the contact angle ($78^\circ$ and $30^\circ$). It is confirmed that the increase of substrate thickness or the decrease of thermal conductivity in a certain range has a reducing effect on the evaporation rate due to the cooling result on the drop. Less heat arrives from the substrate whereas more heat comes from the gas phase. Moreover, a drop on a perfectly conducting substrate ($k_s \to \infty$) evaporates in a similar way as on a solid surface ($e_w \to 0$). However, the semi-infinite substrate ($e_w \to \infty$) is not equivalent to an idealized insulating substrate ($k_s = 0$) which means that the effect of $k_s$ at very small values is not identical to the effect of $e_w$ at very high values. As a consequence, we may say that it is not appropriate to use the thermal resistance of the substrate ($e_w / k_s$) as a common parameter to analyze the effect of thickness and thermal conductivity.
4. Conclusion

Effect of thermal conductivity and thickness of a substrate on which a water droplet evaporates is analyzed numerically by means of the control volume method. A quasi-steady state diffusion model is employed to determine the concentration and temperature fields that are coupled through the saturation concentration as a function of temperature at the drop surface and the heat balance at the liquid-gas interface. The numerical results show that the evaporation rate is between an upper limit corresponding to the case of evaporation on a substrate with a very high thermal conductivity and a lower limit corresponding to the case of evaporation on an ideal adiabatic substrate. The decrease in thermal conductivity of the substrate or the increase of its thickness has the same effect of a greater cooling of the drop and widening the extent of the cold zone due to evaporation.

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