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Analysis of an Evaporating Sessile Droplet on a Non-Wetted Surface

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ABSTRACT

We investigate evaporation of a sessile droplet on a non-wetted surface in the framework of diffusion-limited and quasi-steady evaporation. We extend previous models and numerically solve Laplace equation for the diffusion of liquid vapor into ambient. We propose a unified, simple and accurate expression of the evaporation mass flux valid for $90^\circ \le \theta \le 180^\circ$, where θ is the equilibrium contact angle. In addition, using the derived expression of the evaporation mass flux, we propose a simple and accurate expression of the evaporation mass rate for a non-wetted surface, which does not exhibit singularity at $\theta = 180^\circ$. Finally, using the scaling analysis, the expression of the evaporation mass flux is utilized to estimate the direction and magnitude of the characteristic evaporation-driven flow velocity inside the droplet on a non-wetted surface. The predicted flow direction is found to be consistent with the previous measurements.

Owing to several technical applications, the evaporation of a sessile droplet on a solid surface is a much-studied problem in the interface science in the last decade [1]. In particular, an evaporating droplet can be utilized to self-assemble colloidal particles suspended in it [2]. In the framework of quasi-steady and diffusion-limited evaporation, previous studies [2,3] have shown that the evaporation mass flux (J [kg m^{-2} s]) on the liquid-gas interface is non-uniform on a partially-wetted substrate ($0^\circ < \theta \le 90^\circ$) and the largest evaporation occurs near the contact line. Hu and Larson [3] simplified Deegan's model [2] and provided the following simplified expression of J for a partially-wetted surface,

$$J(r) = J_0(\theta)\left[1 - \left(\frac{r}{R}\right)^2\right]^{-\lambda(\theta)} \quad (1)$$

where r, θ and R are the radial coordinate, contact angle and wetted radius, respectively (Fig. 1(a)). The expressions of $J_0(\theta)$ and $\lambda(\theta)$ are given as follows [3],

$$J_0(\theta) = [D(c_{sat} - c_\infty)/R](0.27\theta^2 + 1.30)(0.6381 - 0.2239(\theta - \pi/4)^2),$$
$$\lambda(\theta) = 0.5 - \theta/\pi \quad (2)$$

where D is the diffusion coefficient [m^2 s^{-1}] of the liquid vapor into outside gas, c_{sat} is vapor concentration [kg m^{-3}] at its saturated value at the ambient temperature, c_∞ is the concentration value in the ambient and R is the wetted radius of the droplet. The evaporation mass flux diverges at the contact line ($r = R$) for $\theta < 90^\circ$ [2,3] and a constant value for $\theta = 90^\circ$ is given by the following expression [4],

$$J = \frac{D(c_{sat} - c_\infty)}{R} \quad (3)$$

The largest error between the numerical solution as compared to the fitted solution obtained by Eq. (1) was around 6% [3].

In case of a non-wetted surface ($90^\circ < \theta \le 180^\circ$), the largest evaporation occurs at the apex of the droplet [5]. The non-wettability or a larger contact angle can be achieved by engineering nano- and micro-textures on a surface with contact angle larger than 65° [6,7]. Popov [4] derived the following generalized expression of J, valid for any contact angle, $0^\circ < \theta \le 180^\circ$.

$$J = \frac{D(c_{sat} - c_\infty)}{R}\left[\frac{1}{2}\sin\theta + \sqrt{2}(\cosh\alpha + \cos\theta)^{3/2}\int_0^\infty \frac{\cosh\theta\tau}{\cosh\pi\tau}\tanh[(\pi - \theta)\tau]P_{-1/2+i\tau}(\cosh\alpha)\tau\, d\tau\right] \quad (4)$$

where α and $P_{-1/2+i\tau}$ are toroidal coordinate and Legendre functions of the first kind, respectively [4]. Stauber et al. [5] revisited solution of an equivalent electrostatics problem reported by Smith and Barakat [8] and derived the following closed form of J for a non-wetted surface at $\theta = 180^\circ$,

$$J(z) = \frac{D(c_{sat} - c_\infty)}{2R_{sph}}\left[1 + \left[\frac{2R_{sph}}{z}\right]^{3/2}\int_0^\infty q\tanh qB_0\left[\frac{rq}{z}\right]\exp(-q)\,dq\right] \quad (5)$$

where $B_0(\cdot)$ is the Bessel function of the first kind of zeroth order, R_{sph} is

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the radius of the sphere fitted to the droplet ($R_{sph} = R/\sin\theta$) and z is the axial coordinate on the liquid-gas interface, expressed as [5], $z = -R_{sph}\cos\theta \pm \sqrt{R_{sph}^2 - r^2}$, where + and − sign corresponds to the upper and lower half of the sphere, respectively. Authors of recent studies [5,9,10] plotted the solution of eq. 4 and showed that the profile of J for a non-wetted surface is significantly different than that for a partially-wetted surface [2,3]. Specifically, in the former, J slightly decreases along the upper half of the droplet and decays to a smaller value near the contact line in the lower half.

The expression of J for non-wetted surface ($90^\circ < \theta \le 180^\circ$) reported in the literature (Eq. (4)) is transcendental and it is not easy to use it in the simple models. A simplified expression of the evaporation mass flux (Eq. (1)) was reported by Hu and Larson [3] for a partially-wetted surface ($0^\circ < \theta \le 90^\circ$). However, to the best of our knowledge, an expression for a non-wetted surface has not been reported in the literature. Similarly, the expression of evaporation mass rate $\dot{M}$ [kg s^{-1}], reported by Hu and Larson [3], is valid for $0^\circ \le \theta \le 90^\circ$ and a simple expression of $\dot{M}$, recently reported by Hu et al. [11], exhibits singularity at $\theta = 180^\circ$. In addition, using scaling analysis, previous studies have shown the dependence of the magnitude of the internal evaporation-driven flow velocity on J on the partially-wetted surface. For instance, the internal flow velocity scales with J near the contact line in the absence of Marangoni stresses [12]. The scaling analysis of the internal flow velocity on a non-wetted surface has not been reported thus far, to the best of our knowledge. Therefore, the objective of this letter is to derive simple and accurate expressions of the evaporation mass flux and evaporation rate of an evaporating sessile droplet on a non-wetted surface ($90^\circ < \theta \le 180^\circ$). A secondary objective is to estimate the direction and magnitude of the internal velocity by scaling analysis, using the derived expression of J.

First, we numerically integrate Eq. (5) to obtain J at $\theta = 180^\circ$ and compare our data with solution of an equivalent electrostatics problem, reported by Smith and Barakat [8]. In this problem, the electrostatic potential field is solved around two perfectly conducting contiguous spheres of the same radius. The vapor concentration and evaporation flux correspond to the electrostatic potential and surface charge density, respectively. Fig. 1(b) shows a good agreement of the variation of normalized evaporation flux ($J_N = JH/[D(c_{sat} - c_\infty)]$, where $H = 2R_{sph}$ is droplet height) with respect to azimuthal angle Φ, obtained in present work and that reported by Smith and Barakat [8]. The direction of Φ is shown in the inset, and $\Phi = 0^\circ$ and $\Phi = 180^\circ$ correspond to the apex of the droplet and to the contact line, respectively. The evaporation flux on the upper hemisphere slightly decreases and the value at $\Phi = 90^\circ$ decreases by 12% of the value at $\Phi = 0^\circ$. In the lower half of the hemisphere, J decays exponentially to zero at $\Phi = 180^\circ$.

Second, a finite element method based numerical model is employed for simulating the diffusion-limited and quasi-steady evaporation of a sessile, spherical cap droplet on a non-wetted surface at ambient temperature (Fig. 2(a)). We solve the diffusion of the liquid vapor in the air surrounding the droplet using Laplace equation [3], $\vec{\nabla}^2 c = 0$, where c is the liquid vapor concentration [kg m^{-3}]. The evaporation mass flux at the liquid-gas interface (J) is expressed as follows, $\vec{J} = -D\vec{\nabla} c|_{LG}$, where subscript LG denotes the liquid-gas interface. We solve the Laplace equation in a computational domain shown in Fig. 2(b). The boundary conditions are shown in Fig. 2(b) and are briefly described as follows. The vapor concentration at the droplet-air interface is prescribed at its saturated value at the ambient temperature ($T_\infty = 25^\circ$C), $c = c_{sat}$. The concentration in the far-field is expressed in term of relative humidity of the ambient (γ) and is given by $c = c_\infty = \gamma c_{sat}$. The value of γ is taken as 0.5 in the simulations. The far-field is set at $r = 50H$, $z = 50H$, where H is the height of the droplet, after performing a domain-size independence study. Axisymmetric boundary condition, $\partial c/\partial r = 0$, is applied at, $z > H$, $r = 0$. No penetration of the vapor concentration into the surface of the substrate, $\partial c/\partial z = 0$, is applied at $r > R$, $z = 0$. The following parameters are used in the model [3]: $D = 2.61 \times 10^{-5}$ m^2/s and $c_{sat} = 2.32 \times 10^{-2}$ kg/m^3. A grid-size convergence study is performed to select adequate grid resolution and a typical grid used in the simulations is shown in Fig. 2(c). The validations of the model are included in the supplementary data.

In the limiting case of $\theta = 180^\circ$, the coordinates of the apex of the droplet are, $r = 0$, $z = H = 2R_{sph}$, $h_N = 1$, where h_N is normalized axial coordinate ($h_N = h/H$). The normalized flux is, $J_N = 2C$, where C is Catalan constant ($C = 0.916$, $2C - 1 = \int_0^\infty q \tanh q e^{-q} dq$), given by Eq. (5) because $B_0(0) = 1$ in this case. The flux, J_N, at the contact line ($h_N = 0$, i.e. $\Phi = 3.14$) is $J_N = 0$, as plotted in Fig. 1(b). Owing to exponential decay of J_N with respect to h_N (Fig. 1(b)), a simplified expression of J_N for $\theta = 180^\circ$ is proposed as follows,

$$J_N(h_N, \theta) = J_0(\theta)[1 - e^{-b(\theta)h_N}]^{-\lambda(\theta)} \tag{6}$$

where J_0, b and λ are functions of θ, and Eq. (6) satisfies $J_N = 0$ at $h_N = 0$. Using curve fitting by least squares method, J_0, b and λ are obtained as $2C$, 5.503 and −1.5, respectively, with $R^2 = 0.998$. In the limiting case of $\theta = 90^\circ$, J_N is constant and equal to 1 (Eq. (3)), and thereby, J_0 and λ are 1 and 0, respectively, in order to extend Eq. (6) to this case.

For $90^\circ < \theta < 180^\circ$, J_N is not zero at $h_N = 0$ (at the contact line) and Eq. (6) cannot be satisfied at $h_N = 0$ for $90^\circ < \theta < 180^\circ$. In order to extend Eq. (6) for $90^\circ < \theta < 180^\circ$ and to alleviate this problem, Eq. (6) is slightly modified as,

$$J_N(h_N, \theta) = J_0(\theta)[k(\theta) - e^{-b(\theta)h_N})]^{-\lambda(\theta)} \tag{7}$$

where J_0, k, b and λ are functions of θ. Note that Eq. (7) is satisfied for $\theta = 90^\circ$ with $J_0 = 1$ and $\lambda = 0$. Using the finite-element model, we performed simulations at different contact angles and contours of the

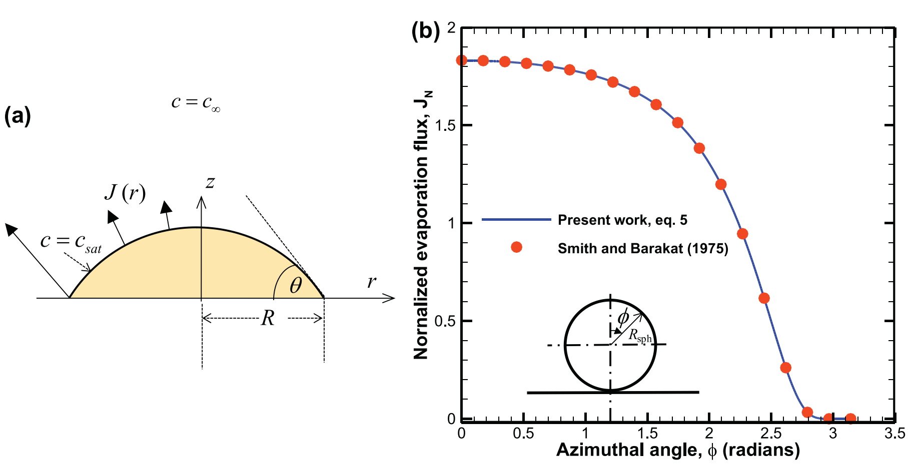

Fig. 1. (a) Geometry of a sessile droplet on a partially-wetted surface (b) Comparison between computed normalized evaporation flux J_N obtained using Eq. (5) for $\theta = 180^\circ$ in the present work and that reported by Smith and Barakat [8] for an equivalent electrostatics problem. The inset shows the geometry of the droplet considered in this case.