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Generalized formulation for evaporation rate and flow pattern prediction inside an evaporating pinned sessile drop

Chafea Bouchenna [a,b,*], Mebrouk Ait Saada [a], Salah Chikh [a], Lounès Tadrist [b]

[a] USTHB, Faculty of Mechanical and Process Engineering, LTPMP, Alger 16111, Algeria
[b] Aix-Marseille Université, CNRS, Laboratoire IUSTI, UMR 7343, 13453 Marseille, France

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ABSTRACT

When a sessile drop is heated from below, it evaporates and it induces a cooling effect in a zone close to the drop surface. The important evaporation rate at the contact line, the surface tension gradient at the liquid-air interface and the buoyancy generate the liquid motion inside the drop. Several parameters affect the evaporation rate among which the substrate properties, the moisture of the surrounding air and the heating conditions. Therefore, different flow patterns could be observed during the evaporation and they are mainly influenced by the relative importance of the evaporation rate, the thermo-capillarity and the buoyancy. The present study uses a generalized formulation to predict the flow patterns at any time during evaporation taking into account all these effects. The contribution and the relative importance of each effect are analyzed under isothermal and non-isothermal heating and different values of the relative humidity of the surrounding air. The correlation proposed by Hu and Larson for assessment of the evaporation rate is extended to non-isothermal surfaces for any evaporation conditions. Flow pattern maps are elaborated based on the dimensionless height of the drop apex and the evaporation conditions.

1. Introduction

The scientific community showed a great interest in the phenomenon of sessile drop evaporation since the last century because of its various applications in metallurgy, biochemical assays, thin film coating, spray cooling, microelectronics, nano-devices and many others. At first, the authors focused on the study of global parameters such as the drop volume, the contact angle and the contact area [1,2]. The failure of some assumptions used in numerical and theoretical predictions, when compared with experimental data, confirms that the sessile drop evaporation is a complex phenomenon. Therefore, to predict reliably this phenomenon, one should include in the analysis all the coupled phenomena, i.e. the heat and mass transfer, the interactions between the solid, liquid and gas phases through different interfaces for a pinned or receding contact line, the evaporation cooling and the fluid flow.

The literature review shows that a tremendous research work was carried out on many aspects of sessile drop evaporation. Recently, Erbil [3] published a review paper about sessile droplets and nearly spherical suspended droplets of micrometer and millimeter size. He reported on research carried out on the topic for about 120 years. He concluded that the imposed parameters like the relative humidity of the surrounding air, the initial contact angle and the imposed temperature have a strong effect on the evaporation rate, the flow field and the temperature distribution. Therefore, it is essential to describe more precisely the operating conditions of the different experiments in order to classify more accurately these works. Cazabat and Guéna [4] presented a general review and some simple cases of analytical solutions existing in the literature to serve as reference for solving problems that are more complex. Larson [5] 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.

The wetting characteristic has been extensively investigated. The published literature shows that the sessile drop evaporation can occur in three different modes: (i) pinned mode with constant contact area and decreasing contact angle, (ii) de-pinned mode where the contact angle remains constant and the contact area decreases, or (iii) stick–slip mode in which both contact angle and contact area decrease with time [6–11]. Birdi and Vu [11]

* Corresponding author at: Aix-Marseille Université, CNRS, Laboratoire IUSTI, UMR 7343, 13453 Marseille, France.

E-mail addresses: bouchennachafea@hotmail.fr (C. Bouchenna), m_aitsaada@yahoo.fr (M. Ait Saada), salahchikh@yahoo.fr (S. Chikh), lounes.tadrist@univ-amu.fr (L. Tadrist).

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Nomenclature

C	concentration (kg/m^3)
c_p	specific heat (J/kg K)
C_v	saturated vapor concentration (kg/m^3)
D	vapor diffusion coefficient (m^2/s)
h_0	height of drop apex (m)
$h_{\alpha,\beta,\phi}$	metric coefficient (m)
$h_{\ell g}$	latent heat of vaporization (J/kg)
Ha	air relative humidity (–)
J	evaporation flux (kg/m^2 s)
Ja	Jacob number (–)
k	thermal conductivity (W/m K)
Le	Lewis number (–)
$\dot{M}$	evaporation rate (kg/s)
Ma	Marangoni number (–)
Ra	Rayleigh number (–)
Ri	Richman number (–)
R_k	thermal conductivity ratio (–)
R_{α_T}	thermal diffusivity ratio (–)
R	contact radius (m)
r, z	cylindrical coordinates (m)
r′, φ	spherical coordinates (m, rd)
T	temperature (°C)
V_D	drop volume (m^3)
u, v	velocity component (m/s)
t	time (s)

Greek symbols

α, β, ϕ	toroidal coordinates (rd)
α_T	thermal diffusivity (m^2/s)
β_T	thermal expansion coefficient (K^{-1})
σ	surface tension (N/m)
ρ	density (kg/m^3)
μ	dynamic viscosity (kg/m s)
ν	kinetic viscosity (m^2/s)
θ	contact angle (°)

Subscripts

s, ℓ, g	solid, liquid, gas
∞	conditions at infinity in surrounding air

Superscripts

*	dimensionless variable

studied experimentally the evaporation of water drop deposited on glass and found that the pinned mode dominates during most of the drop lifetime. Two possible cases were distinguished depending on initial wetting angle for water and *n*-octane drops deposited on glass and Teflon [9–11]. In the case of initial contact angles less than 90°, drops evaporate with a pinned contact line and the evaporation rate varies linearly with time, but in the case of initial contact angle larger than 90°, the evaporation rate is found to be non-linear. Several correlations were proposed to estimate the evaporation rate of sessile drops. In general, they are given as a product of two terms: the first one is a vapor mass diffusion term, and the second one, which has different expressions in the literature, is a function of the wetting angle [1,12–15]. The semi-empirical correlation of Hu and Larson [14] is developed based on the assumption of isothermal drop surface. This correlation does not take into account the substrate nature, the fluid flow and the cooling effect at the drop surface induced by evaporation. Gatapova et al. [16] studied experimentally the evaporation of a water drop on a heated surface with controlled wettability and they developed a simple model of heat and mass diffusion to estimate the specific evaporation rate (evaporation rate per unit surface area). The calculated specific evaporation rates are found in good agreement with experimental data and in qualitative agreement with the correlation of Hu and Larson when considering the vapor concentration on the drop surface. Sefiane and Bennacer [17] proposed a correlation for the evaporation rate including a dimensionless number taking into account the effect of substrate thermal conductivity and thickness. Their results are in good agreement with experimental data. Nevertheless, the expression of the dimensionless number is very complicated, containing parameters not simple to determine accurately.

Another aspect that has been explored by many researchers is the coffee ring phenomenon and the drop stain after evaporation. Undoubtedly, this involves fluid flow inside the drop and the interaction with the surrounding gas for either evaporation mode with a pinned or a receding contact line. Deegan et al. [18] explained the pinned evaporation mode by the liquid motion within the drop assimilated to an outward radial flow to compensate the strong mass loss near the contact line. This outward flow, which was studied experimentally, theoretically and numerically, has a driving effect on the particles contained in drying drops. These particles are carried inside the drop and deposited near the contact line as in the coffee ring phenomenon [19–23]. It is well known that the flow inside the drop is strongly coupled to heat and mass transfer occurring during the evaporation of the drop. The early studies made the assumption of isothermal drop surface until demonstrated that this assumption does not always hold because of the high influence of evaporation cooling at the liquid-gas interface both on the liquid flow and heat transfer inside the drop and on the fluid flow and heat and mass transfer in the surrounding gas [17,24–27]. When the effect of evaporation cooling is considered, a temperature gradient is set at liquid-gas interface and imposes a surface tension gradient inducing thermo-capillary convection [28–33]. This later has a significant effect on drop evaporation and temperature distribution [34,35]. Although, thermo-capillary convection may be induced by heating the substrate or by hot surrounding air or by a very volatile liquid, the present study considers only the case of sessile water droplet in a surrounding air at room temperature. Therefore, thermo-capillary convection may enhance substantially the global evaporation rate in the case of heated substrate, but with negligible effect in the case of non-heated substrate. Moreover, the dependence of fluid density on temperature induces buoyancy convection in the liquid and surrounding gas [35–39], but its importance is still questionable. Some authors demonstrated that buoyancy effect in liquid phase can be neglected in the case where the substrate is at room temperature [40], whereas numerical results of Ait Saada et al. [38] revealed that neglecting buoyancy effect in the gas phase underestimates the evaporation rate especially for heated cases. Carle et al. [41,42] confirmed experimentally that when the substrate is heated, the buoyancy effect in fluid phases must be taken into account in models resolving sessile drop evaporation.

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 [43–45], and the prevalence of one or two effects rules the flow direction inside the drop [8,33,46–48]. Several works were conducted to study the influencing parameters, which define flow patterns in the evaporating sessile drops [40,49–53]. The intensity of thermo-capillary convection depends on temperature gradient along the liquid-gas inter-