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Physics Letters A

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Evaluation of evaporation coefficient for micro-droplets exposed to low pressure: A semi-analytical approach

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ARTICLE INFO

Article history:

Received 5 August 2016

Accepted 27 November 2016

Available online xxxx

Communicated by F. Porcelli

Keywords:

Micro-droplet

Evaporation coefficient

Vacuum

Heat-diffusion

Moving-boundary

ABSTRACT

Evaporation rate of water is strongly influenced by energy barrier due to molecular collision and heat transfer limitations. The evaporation coefficient, defined as the ratio of experimentally measured evaporation rate to that maximum possible theoretical limit, varies over a conflicting three orders of magnitude. In the present work, a semi-analytical transient heat diffusion model of droplet evaporation is developed considering the effect of change in droplet size due to evaporation from its surface, when the droplet is injected into vacuum. Negligible effect of droplet size reduction due to evaporation on cooling rate is found to be true. However, the evaporation coefficient is found to approach theoretical limit of unity, when the droplet radius is less than that of mean free path of vapor molecules on droplet surface contrary to the reported theoretical predictions. Evaporation coefficient was found to reduce rapidly when the droplet under consideration has a radius larger than the mean free path of evaporating molecules, confirming the molecular collision barrier to evaporation rate. The trend of change in evaporation coefficient with increasing droplet size predicted by the proposed model will facilitate obtaining functional relation of evaporation coefficient with droplet size, and can be used for benchmarking the interaction between multiple droplets during evaporation in vacuum.

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1. Introduction

Mass transfer driven cooling mechanism due to evaporation is fundamental in nature, and has a large influence on various applications in the fields of science and engineering. Although evaporation cooling has been applied for numerous industrial and domestic applications, the intensive research in the area still remained inadequate to explain the underlying mechanism to predict evaporation rate accurately. The experimental and molecular dynamic study of evaporation phenomena over the last two decade revealed the existence of an energy barrier in excess to latent heat of evaporation, which has a strong influence on mass transfer rate during evaporation process [1–4].

Among the evaporation cooling techniques, flash evaporation cooling characterized by sudden depressurization of liquid is one of the effective ways of reducing temperature of the liquid rapidly [5]. When the liquid surface is exposed to low pressure, the maximum evaporation mass flux ($\dot{m}''_{e,max}$) in the absence of energy barrier is

derived by Hertz [6] and Knudsen [7,8] by using kinetic theory and is given as follows:

$$\dot{m}''_{e,max} = \sqrt{\frac{M}{2\pi R_u}} \left(\frac{p_s}{\sqrt{T_s}} - \frac{p_v}{\sqrt{T_v}} \right) \quad (1)$$

where, M , R_u , are molar mass of water and universal gas constant respectively, p_s saturation pressure at droplet surface corresponding to surface temperature T_s , T_v is the saturation temperature corresponding to the low pressure p_v maintained in vacuum. However, the presence of energy barrier tends to restrict the evaporation mass flux predicted by Knudsen Eq. (1) [8]. The parameter that captures the restriction on evaporation due to the energy barrier, is called evaporation coefficient (γ_e), and is defined as the ratio of actual evaporation rate to that obtained as the maximum theoretical limit obtained by Eq. (1). For all real purposes γ_e varies within the range [9] $0 < \gamma_e \leq 1$, and observed evaporation mass flux can be obtained as $\dot{m}''_{e,obs} = \gamma_e \dot{m}''_{e,max}$. Extensive studies to determine appropriate value of γ_e over the last few decades produced extremely conflicting results ranging over three orders of magnitude [10,11]. Evaluation of γ_e has a very strong dependence on measurement errors caused significantly by presence of temperature gradient from the surface to the bulk [1], other than due

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<http://dx.doi.org/10.1016/j.physleta.2016.11.036>

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to contamination, uncertainties of surface temperature, and uncertainty of pressure and temperature of vapor just above the surface, to name a few.

In order to verify the range of γ_e at ideal conditions, temperature evolution of micro-droplets of water with radius ranging from 6–20.3 μm exposed of near zero pressure ($< 5 \times 10^{-4}$ Torr), was studied by Smith et al. [12]. The bulk temperature was measured using Raman Thermometry. A simple diffusion based mathematical model [13] was used for obtaining γ_e by fitting γ_e values in the theoretical model to match the experimentally measured temperature evolution. The reason for experiments on such small droplets in high vacuum, was to obtain water molecules to evaporate ballistically (without gas phase collisions [12]), and thus, avoiding the possibility of re-condensation of vapor molecules on the droplet surface. It was also argued that re-condensation can be avoided completely by keeping the droplet size less than the mean free path of the evaporating molecules directly above the evaporating surface [12]. For saturation temperature range 295–273.16 K, the mean free path was found out to be of the order of 10 μm , and almost ideal ballistic or free evaporation can be achieved for droplet radius $r \leq 10 \mu\text{m}$ [12]. The predicted γ_e was reported to be 0.62 ± 0.09 for droplet radius varying within the range from 6 to 20.3 μm .

Interestingly, the prediction of γ_e by lumped heat model was 0.71 ± 0.09 , and greater than that predicted by the diffusion model. Lumped heat model considers infinite heat diffusion rate within the droplet, hence, prediction of droplet cooling rate by lumped model must be faster than that predicted by diffusion model and, a smaller γ_e value is expected to be predicted by lumped model as compared to diffusion model, contrary to the reported prediction by Smith et al. [12].

To address this discrepancy, a close investigation of the phenomena is performed in this present work by developing a rigorous transient heat diffusion model of droplet evaporation cooling. Effect of droplet size reduction due to evaporation from the surface is also considered in the model. However, the effect of size reduction is expected to be negligible, since latent heat of evaporation (h_{fg}) is very large as compared to the small heat content of the droplet.

2. Mathematical modeling

The equation for 1-D heat diffusion in radial direction for a single spherical droplet is given as,

$$\frac{\partial T}{\partial t} = \frac{\alpha}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) \tag{2}$$

where, $\alpha = k/\rho c_p$ is the thermal diffusivity of water. When the superheated droplet enters the vacuum ($p < 5 \times 10^{-4}$ Torr), the droplet is subjected to the following initial and boundary conditions: $T(0, r) = T_i$; $\partial T/\partial r|_{r=0} = 0$; $-k\partial T/\partial r|_{r=r_s} = h_{fg}\dot{m}_e''$, where subscript ‘i’ and ‘s’ designate initial condition and droplet surface respectively. Since the droplet volume decreases due to evaporation from the droplet surface, the rate of change of droplet surface radius can be obtained as: $\rho h_{fg} dr_s/dt = -h_{fg}\dot{m}_e''$. The mass flux can be obtained as: $\dot{m}_e'' = \gamma_e \dot{m}_{e,max}''$, where $\dot{m}_{e,max}''$ is defined by Knudsen Eq. (1) [8] (note: $p_v/\sqrt{T_v} \simeq 0$ for $p_v < 5 \times 10^{-4}$ Torr, and $\dot{m}_{e,max}'' \simeq p_s \sqrt{M/2\pi R_u T_s}$). The vapor pressure at droplet surface p_s can be obtained by using Clapeyron equation for ideal gas using a reference temperature T_{ref} and corresponding saturation pressure p_{ref} , as shown by Eq. (3). The reference temperature considered for the present study is the triple point of water.

$$\frac{p_s}{p_{ref}} = \exp \left[\frac{h_{fg} M}{R_u} \left(\frac{1}{T_{ref}} - \frac{1}{T_s} \right) \right] \tag{3}$$

1-D heat diffusion Eq. (2) is nondimensionalized considering nondimensional temperature $\theta = T/T_i$, radius $r^* = r/r_i$, and time $F_o = t\alpha/r_i^2$ respectively to obtain Eq. (4) with nondimensional initial and boundary conditions: $\theta(0, r^*) = 1$, and $\partial\theta/\partial r^*|_{r^*=0} = 0$, $\partial\theta/\partial r^*|_{r^*=r_s^*} = -H\theta_s$. Nondimensional mass flux (H), and surface temperature are defined as: $H = r_i h_{fg} \dot{m}_e''/kT_s$, and $\theta_s = T_s/T_i$ respectively. Similarly, the rate of change of nondimensional droplet surface radius can be obtained as: $dr_s^*/dF_o = -\dot{m}_e'' r_i/\rho\alpha$.

$$\frac{\partial\theta}{\partial F_o} = \frac{1}{r^{*2}} \frac{\partial}{\partial r^*} \left(r^{*2} \frac{\partial\theta}{\partial r^*} \right) \tag{4}$$

The analytical solution of Eq. (4) can be obtained as [14]:

$$\theta = \frac{4}{r^*} \sum_{n=1}^{\infty} C_n \frac{\sin(\lambda_n r^*)}{e^{\lambda_n^2 F_o}} \int_0^{r_{s,i}^*} \theta(0, r^*) r^* \sin(\lambda_n r^*) dr^* \tag{5}$$

In Eq. (5), λ_n are the positive roots of the transcendental equation $\tan(\lambda_n r_s^*)/\lambda_n r_s^* = 1/(1 - Hr_s^*)$, and, $C_n = \lambda_n/[2r_{s,i}^* \lambda_n - \sin(2\lambda_n r_{s,i}^*)]$.

The transient temperature profile given by the series solution in Eq. (5) can be obtained by using an iterative scheme. The heat flux at the droplet surface is defined by the evaporation flux \dot{m}_e'' , which is a highly nonlinear function of the droplet surface temperature. The iterative procedure involves taking the first guessed value of surface temperature (T_s) at time $t + \Delta t$ to be the surface temperature at time t , and calculating the first guess for \dot{m}_e'' and, hence, H at time $t + \Delta t$. The non-dimensional surface radius r_s^* can also be updated from the first guess of surface mass flux \dot{m}_e'' by numerical integration of equation $dr_s^*/dF_o = -\dot{m}_e'' r_i/\rho\alpha$, over the nondimensional time interval F_o to $F_o + \Delta F_o$. Once, H and r_s^* are calculated, λ_n values can be obtained solving transcendental equation for λ_n , which in turn can be used in Eq. (5) to obtain the next guess of temperature distribution in the droplet including the surface temperature. The iteration continues till r_s^* and T_s converges with error limit less than 10^{-7} .

There are two different ways of treating Eq. (5) numerically: namely, scheme (i) where initial condition $\theta(0, r^*) = 1$ and $r_{s,0}^* = 1$ are used in the integration term of Eq. (5) and obtaining the simplified expression [15] for θ given by Eq. (6), and scheme (ii) where previous time step distribution of $\theta(F_o, r^*)$ and r_{s,F_o}^* are treated as the initial condition for the current time-step ($F_o + \Delta F_o$) and obtaining the integration term in Eq. (5) numerically (Eq. (7)).

$$\theta = \frac{4}{r^*} \sum_{n=1}^{\infty} A_n \frac{\sin(\lambda_n r^*)}{e^{\lambda_n^2 F_o}} \tag{6}$$

$$\theta = \frac{4}{r^*} \sum_{n=1}^{\infty} B_n \frac{\sin(\lambda_n r^*)}{e^{\lambda_n^2 \Delta F_o}} \int_0^{r_{s,F_o}^*} \theta(F_o, r^*) r^* \sin(\lambda_n r^*) dr^* \tag{7}$$

A_n and B_n appearing in Eq. (6) and Eq. (7) are defined as $A_n = [\sin(\lambda_n) - \lambda_n \cos(\lambda_n)]/\lambda_n [2\lambda_n - \sin(2\lambda_n)]$ and $B_n = \lambda_n/[2r_{s,F_o}^* \lambda_n - \sin(2\lambda_n r_{s,F_o}^*)]$ respectively.

Both the numerical schemes described by Eq. (6) and Eq. (7) are implemented to obtain droplet bulk temperature (T_b) evolution and the results are compared with the experimental observation by Smith et al. [12]. Scheme (i) (Eq. (6)), although much simpler to implement, found out to be less accurate as compared to scheme (ii) (Eq. (7)). The reason being quite obvious, and can be attributed to the transient nature of droplet surface boundary condition, as well as the surface location (however small it is). Fig. 1 shows the typical evolution of non-dimensional temperature distribution in the droplet with time for both modeling schemes (i) and (ii). The arrow in Fig. 1 indicates the direction of time. The integration term in Eq. (7) involves numerically obtaining the area

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