Influence of properties of liquidand substrate on evaporation of the sessile drop

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Abstract: - The evaporation of sessile drop investigated as quasi-state-process with mutual influence of temperature and vapor concentration taken into account. Problem was solved numerically, using mathematical model based on finite element method (FEM). The model was tested by comparison its results with experimental ones. The geometry of the droplet leads to nonuniform surface temperature distribution inducing Marangoni thermal flows. We investigated influence of substrate geometry and relative thermal conductivities of substrate and liquid on surface temperature distribution.

Key-Words: -finite elements method; heat transfer; mathematical modeling

1 Introduction

There are plenty technological processes connected with drops drying in different conditions. These technologies used for DNA mapping, lithography, material science, biology, and others.

In earlier studies the flow inside sessile drop was observed and the main reason for flow was considered the nonuniform mass loss from the surface of the droplet [1]. Besides the mass conservation law there are different reasons for inducing and controlling flow inside droplet. Various methods to describe process of drying were created to solve different practical problems such as forming solute deposits with predefined properties or drying of colloidal and biological liquids [2-6].

In some studies stated that under identical conditions flow can be in different directions [7-13]. This phenomenon occurs because evaporation depends on the thermal conductivities of liquid and substrate [14, 15]. Position of the turn point where the flow changes direction, varies for different materials and can be controlled.

Dunn et al. [14, 15] stated that the major factor influencing on evaporation is the size of substrate. They demonstrated differences in temperature's distribution in extreme cases of infinite substrate and drop-sized substrate under thin-drop approximation.

2 Math model

We consider a drop of spherical shape cap resting on the flat solid layer [16]. Under room conditions, the evaporation is a slow process. For instance, the desiccation time of a 15 mg sessile water drop is greater than 3500 s [17]. It allows us to assume a quasi-steady-state process. Thus, the temperature T in substrate and liquid obeys the equation:

$$\Delta T = 0 \quad (1)$$

Outside the drop vapor concentration c satisfies Laplace's equation:

$$\Delta c = 0 \quad (2)$$

We consider bottom substrate boundary at the ambient temperature T_0:

$$T = T_0 \quad (3)$$

On the drop surface the heat flux equals to heat loss due to phase transition of liquid into vapor:

$$k_s(\mathbf{n}\nabla T) = aL(\mathbf{n}\nabla c) \quad (4)$$

where k_s is the substrate thermal conductivity, a is the ambient thermal diffusivity, L is the specific vaporization heat, and $\mathbf{n}$ is the normal vector.

On the droplet surface we consider vapor to be saturated. The concentration of saturated vapor is a strong function of temperature:

$$c = c_0(T) \quad (5)$$

The concentration of saturated vapor and temperature are connected according to [19].

At the boundary between environment and substrate we assume no concentration flow and no heat flow.

$$\begin{cases} \nabla T = 0 \\ \nabla c = 0 \end{cases} \quad (6)$$

On remote boundaries concentration equals to the ambient value:

$$c = c_{amb} \quad (7)$$

At the inner boundary of liquid the continuity of temperature and heat flux conditions take place:

$$\begin{cases} k_s(\mathbf{n}\nabla T) = k_l(\mathbf{n}\nabla T) \\ T_s = T_l \end{cases} \quad (8)$$

where k_s and k_l are thermal conductivities of substrate and liquid, respectively, T_s and T_l are temperatures in substrate and liquid, respectively.

The dimensionless parameters for solution are $k_r = k_l/k_s$ and $r_d/R - 1$, where r_d and R are the drop and the substrate radii, respectively.

The tangential stress τ is

$$\boldsymbol{\tau} = \mathbf{t} \cdot \nabla_s \sigma = \beta(\mathbf{t} \cdot \nabla_s T) \quad (9)$$

where $\mathbf{t}$ is tangential unit vector, σ is surface tension, ∇_s is the surface gradient, and $\beta = \dfrac{\partial \sigma}{\partial T}$ is the material parameter that is negative for most liquids. The direction of Marangoni flow determined by the temperature gradient over the droplet surface.

The local evaporation rate is

$$\mathbf{J} = -D\nabla c \quad (10)$$

where D is the diffusion coefficient, and total volume loss is

$$-\frac{dV}{dt} = \frac{1}{\rho}\int_S \mathbf{J} d\mathbf{S} = -\frac{1}{\rho}\int_S D\nabla c d\mathbf{S} \quad (11)$$

where integration goes over the droplet surface.

The reason why this problem solved numerically is that impossible to separate it into independent ones. The temperature and concentration have strong influence on each other, and there is no analytical solution for such self-conjugated problems. To solve this problem we used the finite elements method (FEM) based on commercial software package, COMSOL Multiphysics 4.3.

3 Case study

To test the created model we examined two extreme cases: substrate size equal to droplet radius andsubstrate is infinite. As example results we used ones acquired by Dunn. Dunn developed two different models [14], each of them is in good agreement with experimental results [15]. Experiment used methanol droplet on substrate of aluminum or PTFE.

In the first model, Dunn considered thin drop approximation, i.e. no horizontal heat fluxes, no horizontal components in equations. Such simplification turns two-dimension Laplace's equation into one-dimensional heat transfer equation. In order to implement such conditions in our model we set substrate size equal to the drop radius. In latter model, there are no restrictions on thicknesses of the droplet and substrate, and horizontal size of the substrate is much greater than the drop radius and can be considered infinite.

Fig. 1-2 show comparison between our and Dunn's results, where symbols correspond to Dunn's results and solid lines to ours.

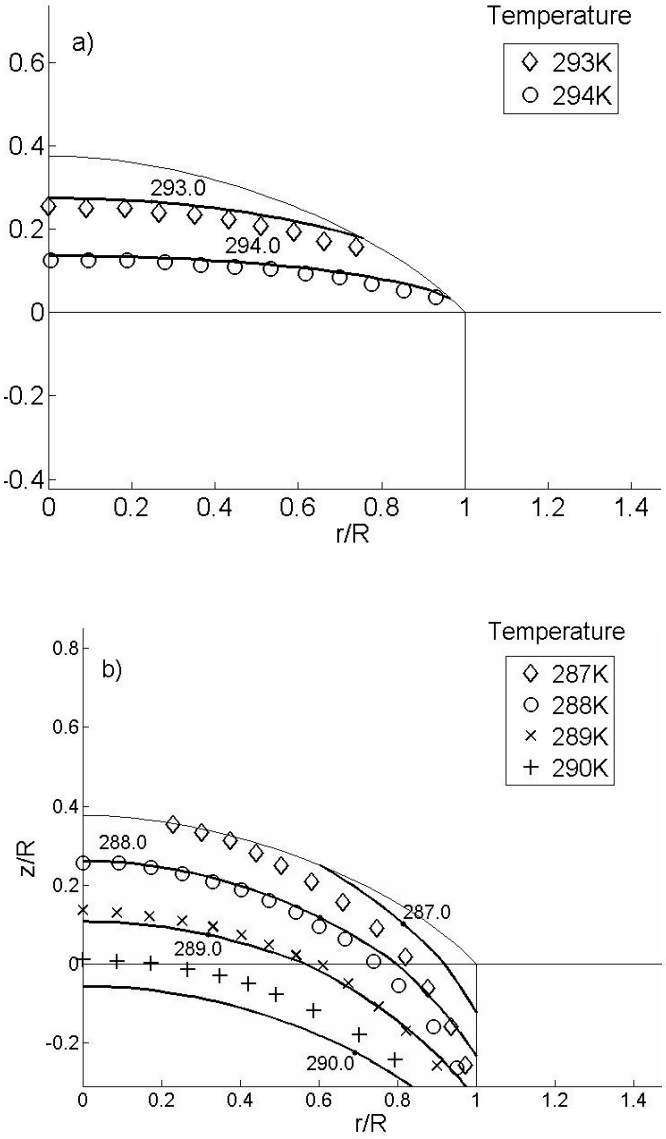

Fig.1. Temperature inside the drop for $r_d = R$ on a) PTFE and b) aluminum

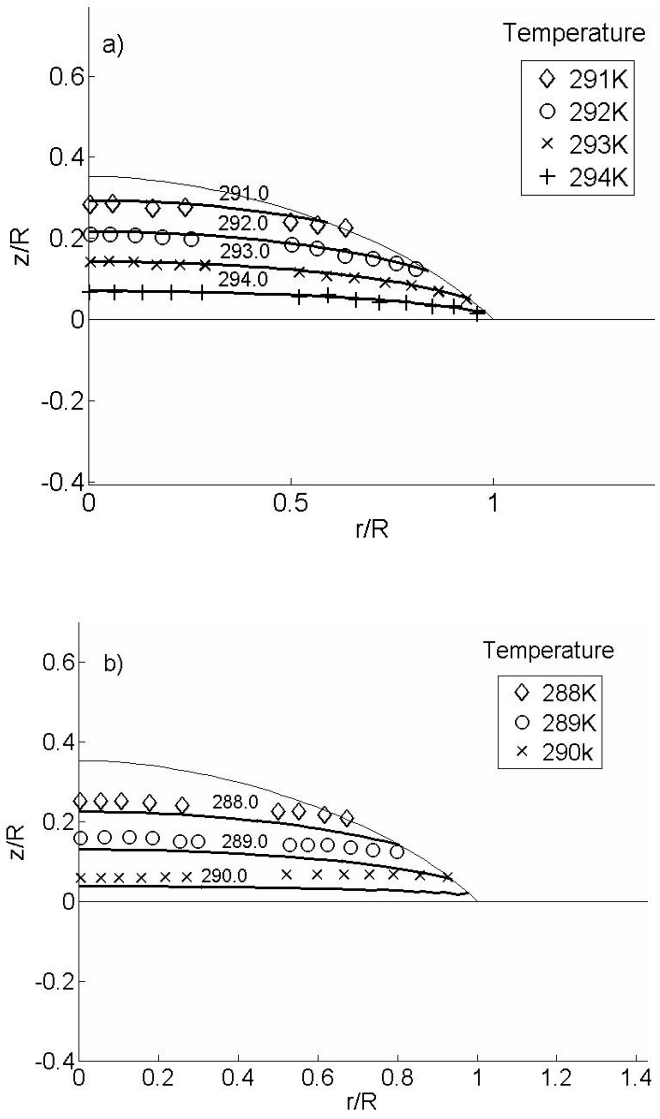

Fig.2. Temperature inside the drop for a) PTFE and b) aluminuminfinite substrate

Results of our model are in good consistency with ones acquired by Dunn.

Also we comparedtotal volume loss in our model with experimental results acquired by David *et al.* [18]. We used infinite substrate to implement conditions of the experiment and acquired evaporation rate by (11). Volume loss is a linear function of the radius of the drop, as stated by Popov *et al.* [21].Fig. 3 shows comparison between our model's results and experimental work.

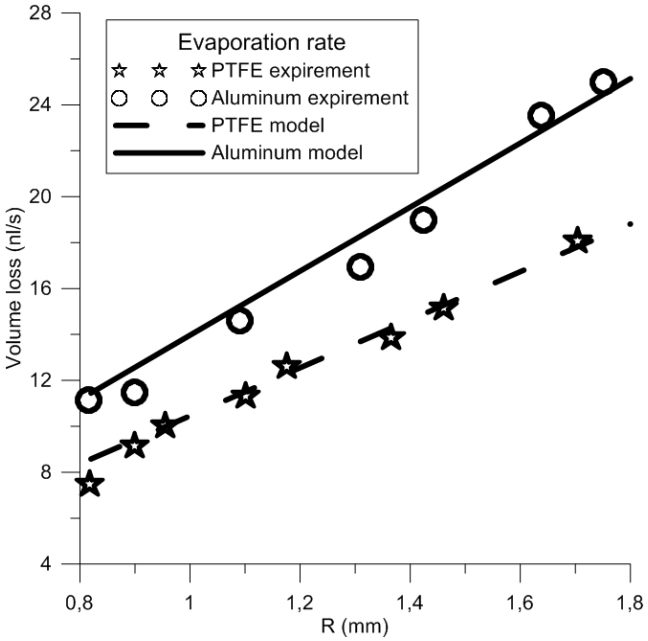

Fig.3. Evaporation rate by model and experiment

4 Results

The heat flux from substrate into the drop is determined by relative thermal conductivity k_s. Due to geometry of the system, more significant variation of heat flux magnitude occurs near the edge of the drop [18]. Fig. 4-6 show temperature deviation on the drop surface:

$$\Delta T = T - T_{top} \tag{12}$$

where T_{top} is temperature on the top of the droplet.

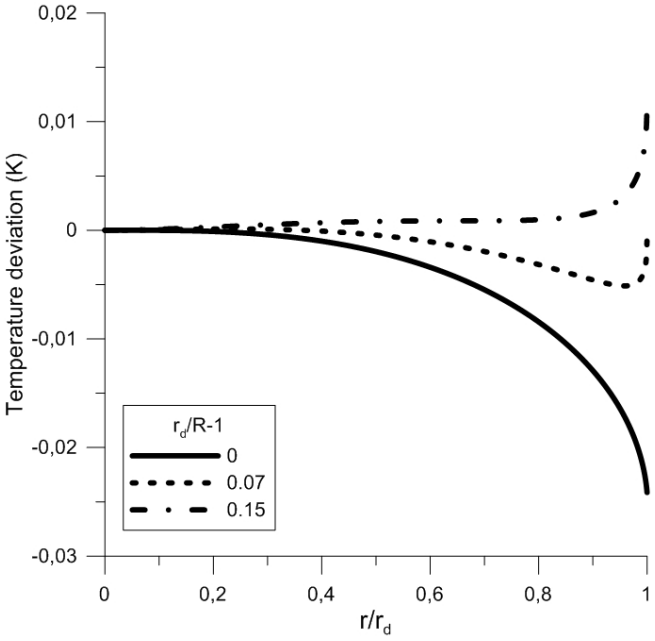

Fig. 4. The surface temperature deviation at $k_r = 0.2$

In case of $k_r = 0.2$ the liquid thermal conductivity is much higher than substrate's. It leads to cooling of the edge of the drop (Fig.4). With variation of substrate size we can increase the heat flux to edge of the drop and thus compensate heat loss due to evaporation.

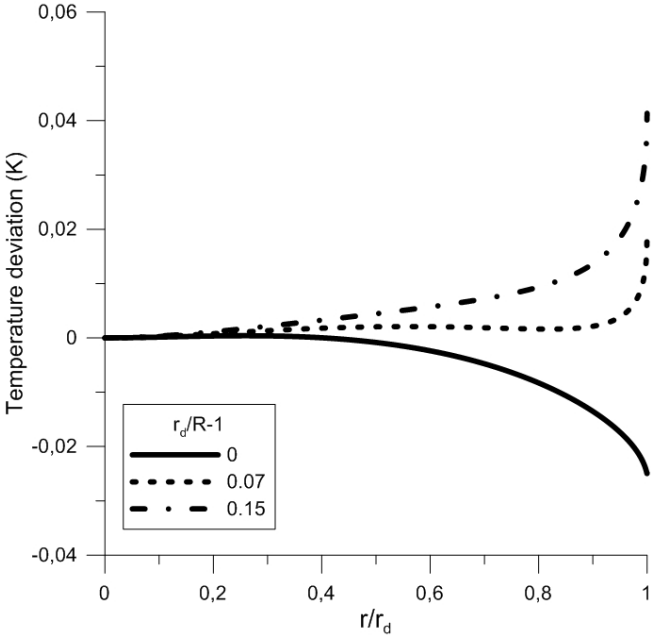

Fig. 5. The surface temperature deviation at $k_r = 0.6$

For $k_r = 0.6$ total heat flux from substrate into the drop is greater than for $k_r = 0.2$. In this case, increasing of substrate size leads not only to compensation of heat loss from the edge, but also to heating significant part of the drop (Fig. 5).

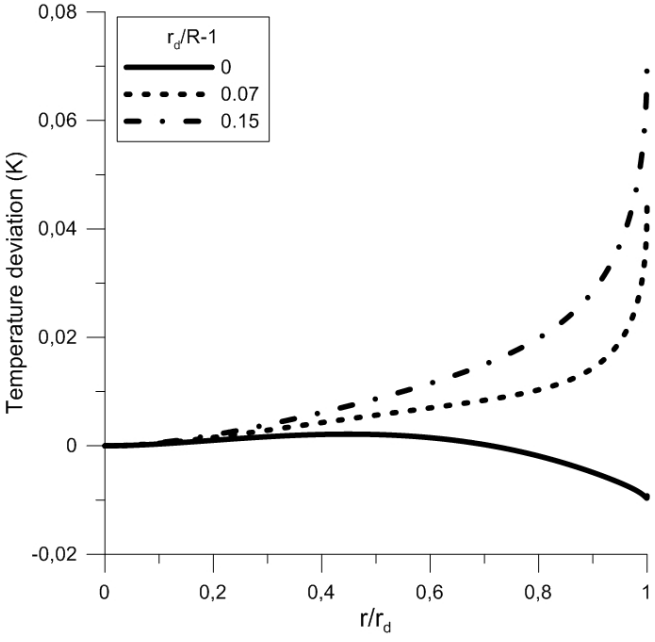

Fig. 6. The surface temperature deviation at $k_r = 1$

With further increasing of k_r the cooling near edge become less than in former cases (Fig. 6). For larger drop size the heat flux from substrate fully compensate cooling due to evaporation and affects entire drop.

5 Conclusion

In this paper we formulated and solved a mathematical model for the quasi-steady diffusion-limited evaporation of an axisymmetric sessile droplet of liquid with a pinned contact line on finite-sized substrate which generalizes the theoretical model proposed by Deegan*et al.* [1] to include the effect of evaporative cooling on the saturation concentration of vapor at the free surface of the droplet, the dependence of the coefficient of diffusion of vapor in the atmosphere and geometry of the substrate. The predictions of the model were found out to be in a good agreement with the recent experimental results.

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