Numerical simulation of the formation of dry spots during film evaporation

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Abstract. This paper presents a developed methodology for calculating heat and mass transfer processes in a cylindrical evaporation cell. The mathematical model reproduces all significant features of the evaporation cell geometry. In this cell, a layer of liquid is formed on a substrate with a diameter of 51 mm, heated below. To simulate heat transfer during film evaporation on a heated substrate, a numerical technique based on the Volume of Fluid method was used. The developed model was used to study the process of dry spot formation during film evaporation. The calculated data are compared with the experiment on the profile of the free surface of the film during evaporation and rupture. In general, results of this testing demonstrated good agreement with experiment. As a result, it was shown that developed numerical method makes it possible to describe process of formation dry spots.

1. Introduction

In connection with problem of global warming and active transition to "green" technologies, tasks of energy conservation and intensification of heat and mass transfer processes get new importance. In this series, an important place is taken by problem of studying processes of evaporation and boiling liquids and increasing their efficiency. These tasks are particularly relevant for solar energy [1]. In spite of high potential for use solar energy, its use remains at a low level. One of these directions is evaporation systems based on conversion of solar energy into thermal energy for implementation of liquid-vapor phase transition [2-3]. These systems perform various functions such as desalination of seawater, power generation, separation of liquids, cleaning of polluted water, etc. However, efficiency of such systems is rather low. And therefore, search for new ways to intensify evaporation processes is an important task, relevance of which is determined by desire to increase efficiency of heat exchange devices in combination with desire to reduce energy costs and achieve maximum compactness with minimum material consumption. To intensify heat transfer process, it is advisable to reduce thickness of liquid layer. However, thin liquid films are prone to rupture, including due to the Marangoni effect. There are a number of studies describing thermocapillary breakdown of liquid films [4-13]. It should be noted that liquid film rupture is closely related to physics of contact line [14-16], which is responsible for behavior of a dry spot after its nucleation.

Study of evaporation processes has a long history starting with works by Thomson [17], Marangoni [18] and Bernard [19]. Since, a fairly large number of various models of these processes have been created [19-26]. In first works on this topic, evaporation processes were usually not taken into account and were limited only to effects of surface tension, including the Marangoni effects. The so-called
single-layer model of thin films is widely used, in which hydrodynamics and heat transfer are calculated only within liquid phase, sometimes involving conjugate heat transfer with a solid substrate. Typical examples of such models can be found in [20]. Processes of flow and heat transfer occurring in gas phase are not taken into account and are modeled by setting appropriate boundary conditions at liquid-gas interface. Two-layer models have become prevalent, in which equations of motion and heat transfer are solved simultaneously for liquid and gaseous media [21, 22]. In recent years, computational models have been actively developing, which make it possible to describe in detail line of contact, including effect of partial wetting of the surface. Thus, in [23], the film evaporation process was modeled by solving Lattice Boltzmann method. Apparently, this approach should be considered as very promising for such tasks. Another class of models that make it possible to simulate the joint flow and heat transfer of gas and films is conjugate model of thin films Eulerian Wall Film (EWF) [24]. In this approach, modeling of a two-phase flow is described using conjugation of a spatial model of gas movement and a flat (within wall) model of film movement.

The above is a quick overview of models and approaches to calculating film evaporation process shows that despite a large number of works on topic under consideration, problem of creating a reliable and universal mathematical model of processes of liquid evaporation at the interface with a moving contact line is still very actual.

Therefore, this work presents results of development of a method for calculating processes of heat and mass transfer during evaporation of a film on a heated substrate, taking into account evaporation.

2. Experimental setup

A horizontal liquid layer is in the experimental cell. The substrate is made of stainless steel and is a disc 51 mm in diameter and 1 mm thick, which is pressed against the base by a polytetrafluoroethylene ring with an inner diameter of 46 mm. The base is a piece of textolite, in the center of which there is a built-in copper rod with a diameter of 12 mm, heated from below by an electric heater. A copper cooling circuit is built around the perimeter of the base, the temperature of which is kept constant by pumping water with a predetermined temperature of 23°C. The power of the electric heater automatically increases by 0.15 W every 18 seconds, as a result, the temperature of the surface of the rod, which is in contact with the substrate and is measured by a thermocouple, smoothly increases.

Water was used as a working liquid, which was prepared using a Milli-Q purification system. The temperature and humidity of the ambient air during the experiment were 23-25°C and 28–30%, respectively.

An IFS2405-3 confocal sensor manufactured by Micro-Epsilon Company was used to point-measure the thickness of the liquid layer. To record the rupture process, a Photron Fastcam high-speed camera was used together with an optical schlieren system, the scheme of which is presented in [25]. The shooting parameters were as follows: shooting speed 3000 frames per second, field of view 23 × 23 mm, image resolution 1024 × 1024 pixels.

Figure 1. Schematic of the experimental setup.
3. Numerical model

A mathematical model of the evaporation system described above was developed. The model reproduces all significant features of the evaporation cell geometry. In this cell, a layer of liquid is formed on a substrate with a diameter of 51 mm, which is pressed by teflon ring to base of working area. In the center, substrate heats up, along perimeter it cools. Heat flux increases smoothly until film breaks. Substrate is heated at a rate of approximately 1.5 °C per minute. The geometry of the computational domain (Figure 2) consists of a copper cylindrical heater, a textolite base, a stainless steel substrate, and a free space above substrate, in which film is placed. The problem under consideration makes it possible to use an axisymmetric formulation. The experiments carried out have shown that this approximation is performed with good accuracy. It is well known that the problem of direct modeling requires sufficiently detailed computational meshes to resolve the interface between the phases of newly formed small droplets and films. To solve this problem, technology of gradient adaptation of computational mesh was used. With help of this technology, computational mesh in calculation process is automatically refined in area of large solution gradients. In this case, gradient of liquid volume fraction is used as a control parameter. The mesh cells in interface area can be four to sixteen times smaller than in original mesh (Figure 2b). Due to this technology, it is expected to obtain a solution acceptable in terms of accuracy on computational meshes that are reasonable of detailing. Another very important problem of methods for solving tasks with a free surface is artificial blurring and deformation of interface associated with numerical errors arising when solving the Euler equation of transfer for volume fraction of liquid in cells. Currently, this problem is solved mainly in two ways. In the first method, solution of convective transport equation is carried out on basis of so-called geometric reconstruction schemes, in which phase boundary in computational cell is approximated using geometric surfaces. For example, by constants, as in classical donor-acceptor scheme of Hirt, or by straight lines (planes in 3D) as in later works of Young (PLIC (piecewise linear interface construction) scheme) and Rudman. The good thing about geometric reconstruction is that it does not allow free surface of the liquid to "spread" over more than one cell of computational mesh. The thickness of interface in such schemes is strictly defined. However, from a computational point of view, these schemes are extremely expensive and difficult to implement, especially in a three-dimensional case. In addition, it is well known that this kind of scheme has serious problems associated with conservation of liquid mass, which arise at stage of reconstruction (cutting off) of interface in computational cell. For these reasons, recently, use of TVD (total variation diminishing) and WENO (weighted essentially non-oscillatory) schemes has been considered as a real alternative to such schemes for solving convective transport equation within framework of VOF (volume of fluid) methods. As is known, class of TVD schemes was specially developed to solve discontinuous equations of gas dynamics. TVD schemes are designed to resolve shock waves for no more than a few computational cells. The experience of using TVD schemes to solve convective equation of volume fraction transfer in a computational cell showed that these schemes reproduce deformation of interface, in general, no worse than schemes with geometric surface reconstruction, but at same time they are much more conservative and require several times less time to solve. Therefore, TVD schemes with various limiters have recently become widely used for modeling problems with a free surface. In this work, the HRIC (high resolution interface capturing scheme) limiter was used for these purposes.
To simulate heat transfer during film evaporation on a heated substrate, a numerical technique based on the Volume of Fluid method was used. The model is based on our works [25-26]. Below are the basic equations of this model.

The mass conservation law for a two-phase media takes the form:

\[
\frac{\partial}{\partial t} (\rho_v \alpha_v) + \nabla \cdot (\rho_v \alpha_v \mathbf{v}) = S_v
\]

(1)

Where \( \alpha_v \) – volume fraction of vapor, \( \rho_v \) – vapor density

The volumetric source of vapor during evaporation was determined according to model of Lee et al.

\[
S_v = r \alpha_i \rho_l \frac{T - T_{sat}}{T_{sat}} \quad (T > T_{sat})
\]

(2)

where \( r \) – empirical mass transfer intensity factor, \( \alpha_i \) – volume fraction of liquid, \( \rho_l \) – liquid density, \( T_{sat} \) – the saturation temperature.

Density, viscosity, thermal conductivity and heat capacity of the media are determined as follows:

\[
\rho = \alpha_i \rho_l + \alpha_v \rho_v
\]

\[
k = \alpha_i k_i + \alpha_v k_v
\]

\[
\mu = \alpha_i \mu_i + \alpha_v \mu_v
\]

\[
C_p = \frac{\rho \alpha_i C_{p,v} + \rho \alpha_v C_{p,l}}{\rho \alpha_v + \rho \alpha_i}
\]

The momentum conservation equation has a standard form:

\[
\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \left[ \mu \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) \right] + \rho g + F_s
\]

(3)

where \( F_s \) – interfacial tension force. Continuum surface force algorithm was applied to simulate interfacial tension.
\[
F_{s_{\text{w}}} = \sigma_{iv} \frac{\alpha_{v} k_{v} \nabla \alpha_{v} + \alpha_{v} \rho_{v} k_{v} \nabla \alpha_{v}}{0.5 \left( \rho_{l} + \rho_{v} \right)}
\]  
(4)

\[
k_{v} = -k_{l} = -\nabla \cdot \left( \frac{\nabla \alpha_{v}}{\nabla \alpha_{l}} \right)
\]  
(5)

where, \(\sigma_{iv}\) – interfacial tension coefficient between two phases.

The energy conservation equation has the form:

\[
\frac{\partial}{\partial t} \left( \rho E \right) + \nabla \cdot \left[ \nu \left( \rho E + p \right) \right] = \nabla \cdot \left[ k \nabla T \right] + S_{h}
\]  
(6)

\[
E = C_{p} \left( T - T_{\text{sat}} \right)
\]  
(7)

where \(S_{h} = -L \cdot S_{v}\), \(L\) – heat of vaporization.

Boundary conditions: nonslip conditions were set on all walls in contact with liquid. Free exit conditions were set on upper edge of computational domain. On lower edge of heated cylinder, heat flux density was set corresponding to experimental conditions. On side walls of computational domain, heat transfer conditions were set corresponding to free convection in air. The dynamic wetting angle was simulated using the model described in [27].

4. Results

To test this method, we simulated process of water evaporation in cell under consideration. Thickness of liquid film at initial moment of time was equal to 500 µm. Heating power was 75 W. At initial moment, film had a uniform thickness and was at rest. Under these conditions, the film cannot be uniform. Its deformation begins very quickly, associated with the action of surface tension forces and free convection. And the film thickness changes during the calculation. This is also observed experimentally. The model also describes these processes. Evolution of free surface of film during its evaporation and movement under action of interfacial tension forces caused by the Marangoni effects are shown in Figures 3a. Film is shown in red. At initial moment of time, because of evaporation, film is deformed in central part. The film thinning quickly. Surface of film above heater has a parabolic shape. Then film breaks. Then surface of heater is dried. Figures 3b on the right show distribution of temperature isolines in substrate and film. It is seen that availability of a film and its evaporation have a significant effect on temperature distribution.
Figure 3. Motion of a water film after its break (a) and distribution of temperature field in central section of computational domain (b) at different time step. From top to bottom 0.0009 s, 0.0059 s, 0.0019 s, 0.043 s, 0.066 s and 0.1 s.

Figure 4 shows a comparison of calculated data with experiment on growth of dry spot diameter during film evaporation. In the experiment, dependence of diameter on time was obtained using video image processing. As we can see, calculation at initial stages of spot growth reproduces well experimental data. For large spots, calculation slightly overestimates their size.
5. Conclusions
In this work, a mathematical model of a cylindrical evaporation cell has been developed. The model is based on liquid-in-cell method and takes into account thermocapillary effects. A series of test calculations was carried out in which influence of various parameters of model on correctness of modeling process of formation dry spots in process of film evaporation was investigated. As a result, it was shown that developed numerical method makes it possible to describe process of formation of dry spots. Comparison of calculated data with experiment on shape of the free surface of film in process of evaporation and break, on dynamics of motion of contact line with an increase in spot size is carried out. In general, the results of this testing demonstrated good agreement with experiment.

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