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NUMERICAL MODELING OF THERMOCAPILLARY DEFORMATIONS IN LOCALLY HEATED LIQUID LAYER

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Abstract The problem of thermocapillary deformation of the locally heated horizontal liquid layer is considered. The numerical solution of the problem has been obtained in the lubrication approximation theory for two-dimensional axisymmetric thermocapillary flow. The model takes into account surface tension, viscosity, gravity and heat transfer in the substrate and liquid. Evaporation is neglected. The numerical algorithm for the joint solution of the energy equation and the evolution equation for the liquid layer thickness has been developed. Stationary solutions have been obtained by the establishment method. There have been measured and numerically calculated deformations in locally heated horizontal layers of silicone oils of different types and thickness. The dependencies of the depth of thermocapillary deformations on the layer thickness have been obtained for silicone oils of different viscosities. It has been found that the value of the relative deformation of the layer decreases nonlinearly with increasing the layer thickness, when other conditions being equal. It has been found a good qualitative agreement of numerical results and experimental data.

Key words: thermocapillary effect, deformations of the liquid surface, silicone oil, lubrication approximation theory, energy equation, method of fractional steps.

AMS Mathematics Subject Classification: 76B45, 76A20, 76D08, 80A20, 76M12, 35K55.

1 Introduction

At the present time a great attention is paid to the study of mechanisms that lead to the dynamic deformations of the liquid-gas interface. Studying the dynamics of deformations in the horizontal liquid layers under the local heating is a challenge of technological processes, since thin films provide a high intensity of heat and mass transfer. Moreover, thin liquid films are widely used in various systems and apparatus, for example, in heat pipes, evaporators, condensers, cooling systems for electronic equipment. Apart from this, film flows are specially created in various devices of chemical technology, food and pharmaceutical industry.

In systems with a liquid-gas interface one of the main role is played by thermocapillary flows that can be caused even by slight inhomogeneities in the temperature of the interface [1-4]. It is perspective to use the thermocapillary effect when the thin layers of liquid are heated locally to determine the properties of the liquid and the thickness of the layer [5, 6]. Thermocapillary phenomena in thin films lead to deformation of the free liquid surface [7].

In most theoretical works processes in thin liquid layers are modeled using an evolution equation for the layer thickness obtained in the lubrication approximation theory (long-wave approximation) [8]. Velocity, temperature, pressure of the liquid, etc. are defined as a function of film thickness (the solution of this equation). This approach eliminates the complexity of the problem caused by the presence of the free surface.

The aim of investigation and tasks of this work are the theoretical study of thermocapillary deformations in the locally heated horizontal liquid layers with different properties and numerical modeling based on the thin layer approximation, creating of the basis for solving the inverse problems of thermocapillary convection (determination of the thermophysical coefficients of the investigated liquid); comparison of calculation results with available experimental data.

2 Physical statement of the problem

A thin horizontal liquid layer of silicone oil under the local heating is considered, Fig.1. Heater is a thin uniform heat source. Local heating of the liquid layer occurs from the substrate side. The geometry and conditions of the investigated system are axisymmetric. Initially the temperature of the entire system is constant. At the initial moment of time the heater is turned on, and the cuvette and liquid start to warm up. There is a tangential stress on the surface of the liquid, caused by the inhomogeneity of its temperature. Thermocapillary flow and deformation of the liquid surface are formed.

3 Numerical modeling

The problem of thermocapillary deformation of the locally heated horizontal layer of silicone oil with free surface has been solved using the lubrication approximation theory for two-dimensional axisymmetric statement. The model takes into account important parameters such as gravity, surface tension, capillary pressure, thermocapillary effect, viscosity, heat transfer in the substrate and liquid. Evaporation is neglected. Initially the liquid layer has flat surface and uniform temperature. The substrate is locally heated from the bottom side. Deformations of the liquid surface are determined by the properties of the liquid, substrate and heater. Stationary solutions have been obtained by the establishment method. Dynamics of thin films is well described by the evolution equation, which has been obtained using the lubrication approximation theory [8,10,11]:

$$h_t + divq = 0 \tag{1}$$

where h is film thickness, h_t is velocity of the surface motion, $q = \frac{h^3}{3\mu}f + \frac{h^2}{2\mu}\tau$ is vector of local liquid flow rate along the surface, $f = grad(\rho g h + \sigma H)$ is pressure gradient, $\tau = \sigma_T gradT$ is thermocapillary tangent stress, μ is coefficient of dynamic viscosity, ρ is density of the liquid, g is gravitational acceleration, σ is surface tension, σ_T is surface tension temperature coefficient, T is temperature, $H = \frac{h_{rr}}{(1+h_r^2)^{3/2}} + \frac{h_r}{r(1+h_r^2)^{1/2}}$ is double mean curvature of the liquid surface, where h_r and h_{rr} are the first and the second order derivatives with respect to r.

Substituting expressions for the curvature of the surface and the vector of the local flow rate we obtain the equation in cylindrical coordinates for the axial symmetrical case:

$$h_t + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left[\frac{h^3}{3\mu}\frac{\partial}{\partial r}(\rho g h + \sigma H) + \frac{h^2}{2\mu}\sigma_T\frac{\partial T}{\partial r}\right]\right) = 0 \tag{2}$$

Equation (2) is a nonlinear differential equation of the first order in time and the fourth order in spatial variables relative to unknown function $h(t, r)$.

Boundary conditions for equation (2) have a clear physical meaning. Here, R_c is a cuvette radius, t is time.

- $h_r(t, 0) = 0$ the condition of the axial symmetry in the center of the cuvette;
- $h_r(t, R_c) = 0$ the contact angle is given on the border of the cuvette;
- $q(t, 0) = 0$ flow rate is equal to 0 in the center;
- $q(t, R_c) = 0$ the condition of impermeability of liquid through the walls.

The temperature of the liquid layer and cuvette is determined by the energy equation in cylindrical coordinates:

$$\rho C_p\left(\frac{\partial T}{\partial t} + u\frac{1}{r}\frac{\partial(rT)}{\partial r} + \nu\frac{\partial T}{\partial z}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(\lambda\left(r\frac{\partial T}{\partial r}\right)\right) + \frac{\partial^2 T}{\partial z^2} + Q \tag{3}$$

where λ is coefficient of thermal conductivity, C_p is specific heat of the medium (solid or liquid), ρ is density of the liquid, u, v are components of the velocity vector, Q is bulk density of the heat sources, $Q = Q(r, t, z) = \begin{cases} 0, \text{ outside heater} \\ const > 0, \text{ on heater} \end{cases}$.
The heated surface is as a thin circular layer in the center of the cuvette bottom with heater radius R_h, where absorption of laser beams takes place.

Boundary conditions for equation (3) have form:

- $\frac{\partial T}{\partial r}\mid_{r=0} = 0$ axial symmetry condition;
- $\frac{\partial T}{\partial r}|_{r=R_c} = 0$ adiabatic right side wall;
- $\frac{\lambda \partial T}{\partial n}|_W = \alpha_w(T_W - T_a)$ convective heat transfer coefficient is specified on cuvette bottom;
- $\frac{\lambda \partial T}{\partial n}|_S = \alpha(T_S - T_a)$ convective heat transfer coefficient is specified on free liquid surface.

Index W determines the conditions at the bottom of the cuvette, index S determines the conditions on the free liquid surface, α is convective heat transfer coefficient, T_a is ambient temperature, n is normal vector to the surface.

Initially liquid surface is flat and temperature of the liquid surface and cuvette is uniform:

$$h|_{t=0}(r, z) = h_0, T|_{t=0}(r, z) = T_0 = const \tag{4}$$

4 Calculating method

For calculations there has been used splitting into physical processes, such as thermal conduction and liquid motion. The grid in the space variables in the liquid and solid phases is uniform: $r_i = i \cdot dr$, $i = 0, .., N$, $z_j = j \cdot dz$, $j = 0, .., M$ where dr and dz are space steps in r and z directions correspondingly. Number of points in space for numerical calculations is ($N + 1$ x $M + 1$). The time step dt is constant. The value of the liquid layer thickness in the time t_k and node i is $h_i^k = h(r_i, t_k)$.

The evolution equation of the liquid layer thickness (2) is approximated at grid's nodes with finite volume method [11] with an implicit finite-difference scheme of first order in time and of second order in space [9, 10]. The implicit scheme is chosen to ensure stability [11]. A discrete analogue of eq. (2) is written for each volume V_i:

$$\frac{h_i^{k+1} - h_i^k}{dt} + \frac{1}{r_i}\frac{q_{i+1/2}r_{i+1/2} - q_{i-1/2}r_{i-1/2}}{dr} = 0 \tag{5}$$

Expression for approximation of the vector of local liquid flow rate along the surface $q = \frac{h^3}{3\mu}f + \frac{h^2}{2\mu}\tau$ is following:

$$q_{i+1/2} = \frac{(h_{i+1/2}^{k+1})^3}{3\mu}\frac{(f_i^{k+1} - f_{i+1}^{k+1})}{dr} + \frac{(h_{i+1/2}^{k+1})^2}{2\mu}\tau_{i+1/2}^{k+1}. \tag{6}$$

Here pressure f is expressed in such way:

$$f_i^k = \rho g h_i + \sigma H_i; \tag{7}$$

thermocapillary tangent stress is

$$\tau_{i+1/2} = \sigma_T \frac{(T_i + T_{i+1})}{dr}; \tag{8}$$

double mean curvature of the liquid surface H contains the first and the second order derivatives of liquid layer thickness, which approximated in such way:

$$h_{r,i} = \frac{h_{i+1} - h_{i-1}}{2dr}, h_{rr,i} = \frac{h_{i+1} - 2h_i + h_{i-1}}{dr^2}; \tag{9}$$

and approximation of layer thickness is:

$$h_{i+1/2} = \frac{h_i + h_{i+1}}{2}. \tag{10}$$

The system of nonlinear algebraic equations (5) obtained in the approximation is solved at each time step by the Newton's method, and the Jacobians are calculated using numerical linearization [9, 10]. The scheme has the second-order approximation for the spatial coordinates and the first-order in time.

For calculating the temperature in the liquid, deformations of the surface are not taken into account. Since the heater is thin, we assume that the heat source is concentrated only in one layer of nodes. The energy equation (3) is approximated by a finite difference scheme using the fractional step method [11]:

$$\begin{cases} \frac{T_{ij}^{n+1/2}-T_{ij}^{n}}{dt} = \frac{\lambda}{2\rho C_p}\left(\frac{\left(1+\frac{dr}{2r}\right)T_{i+1,j}^{n+1/2}-2T_{ij}^{n+1/2}+\left(1-\frac{dr}{2r}\right)T_{i-1,j}^{n+1/2}}{dr^2}+\frac{T_{i,j+1}^{n}-2T_{ij}^{n}+T_{i,j-1}^{n}}{dz^2}\right)+\frac{Q_{ij}^{n}}{2\rho C_p} \\ \frac{T_{ij}^{n+1}-T_{ij}^{n+1/2}}{dt} = \frac{\lambda}{2\rho C_p}\left(\frac{\left(1+\frac{dr}{2r}\right)T_{i+1,j}^{n+1/2}-2T_{ij}^{n+1/2}+\left(1-\frac{dr}{2r}\right)T_{i-1,j}^{n+1/2}}{dr^2}+\frac{{}_{i,j+1}^{n+1}-2T_{ij}^{n+1}+T_{i,j-1}^{n+1}}{dz^2}\right)+\frac{Q_{ij}^{n}}{2\rho C_p} \end{cases},$$

where $Q_{ij}^n = \begin{cases} \frac{P}{\pi R_h^2 dz} & \text{at } i < \frac{NR_h}{R_c}, j = M/2+1, \\ 0 & \text{for others i, j.} \end{cases}$, here P is given value of the heater power, R_c is cuvette radius, R_h is heater radius.

Boundary and initial conditions are set in the finite differences equations:

- $T(j,0) = T(j,2)$, $j = 1,..,M$ symmetry condition;
- $T(j,N+1) = T(j,N-1)$, $j = 1,..,M$ adiabatic right wall;
- $T(0,i) = T(2,i) - \alpha/\lambda(T(1,i) - T_a)2dh$, $i = 1,..,N$ heat transfer coefficient on the liquid surface;
- $T(M+1,i) = T(M-1,i) - \alpha_w/\lambda_w(T(M,i) - T_a)2dh_w$, $i = 1,..,N$ heat transfer coefficient on the cuvette bottom.

Initial conditions: $T_{i,j}^0 = 0$, $i = 0,..,N$, $j = 1,..,M-1$.

The obtained systems of linear algebraic equations at each step were solved by the tridiagonal matrix algorithm. Problem's data satisfies sufficient conditions for determining the correctness and stability of tridiagonal matrix algorithm. The numerical algorithm for the joint solution of the energy equation and the evolution equation for the liquid layer thickness has been developed. The calculations are performed sequentially. The time step for the evolution equation is done after the time step for the energy equation. Since the process of heat conduction is much slower than the changings in the layer thickness, there are no problems in combining such steps. The mathematical model accounted such defining parameters as the geometry of the problem, parameters of the liquid (table 1), properties of the substrate and the heater materials, heating methods. The calculation results have shown that all these parameters have a significant impact on the distribution of the heat and deformations of the liquid surface.

Table 1: Properties of silicone oils of different types, temperature condition $T = 20^0C$

oil type	σ, N/m	σ_T, N/(m·K)	ρ, kg/m^3	C_p, J/(kg·K)
PMS-5	18.27	-0.066	911.4	1640
PMS-50	19.24	-0.052	960	1549

5 Analysis of calculation results

Comparisons with experimental data [13] have been made. Thermocapillary deformation of dimethylpolysiloxane layer (PMS or silicone oil) was investigated using laser scanning confocal microscope Zeiss LSM 510 Meta. This microscope allowed obtaining highly accurate data on thermocapillary deformation at the stage of steady flow. Experimental measurements were conducted for five types of silicone oil: PMS-5, PMS-50, PMS-100, PMS-200 and PMS-400.

Initial thickness of silicone oil is of the order of several hundred micrometres. The taken types of silicone oil cover the range of viscosity from 5 to 365 cP, other thermal properties are slightly varied. Heater power is $Q = 16.5 \pm 5$ mW.

The experimental scheme is shown in Fig.1. One of the special feature of experimental setup was that the bottom of glass cuvette was colored with a layer lacquer based on nitrocellulose. The lacquer coating was transparent to the beam of scanning microscope,thus, absorbed about 99% of the semiconductor laser. In this way the bottom layer was induced by the heat source (heater).

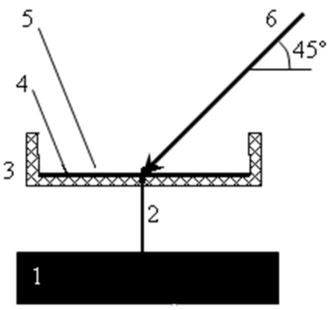

Figure 1: The experimental scheme. 1 microscope lens, 2 scanning beam microscope (wavelength $\lambda = 488$ nm), 3 glass cuvette (cuvette radius $R_c = 18$ mm), 4 layer of colored lacquer based on nitrocellulose, 5 layer of silicone oil, 6 ray semiconductor laser (wavelength 650 nm, power $P = 16.5 \pm 0.5$ mW).

Dependencies on the silicone oil thickness of the thermocapillary deformation's depth have been measured experimentally and calculated by the model (Fig.2). Numerical calculations were made for two marks of silicone oil: PMS-5 and PMS-50.

The depth of the thermocapillary deformation depends strongly on the initial thickness of the layer and the oil viscosity. The thinner the layer, the greater the difference Δh, when other things being equal. In thin layers thermocapillary deformation depth reaches 30% or more of the initial thickness, but quickly decreases with increasing h_0 (see Fig.3). When the layer thickness is $h > 400$ μm values of deformations are practically the same, because viscosity variations for thick layers have less effect on the value of deformation. There is a good qualitative agreement between the calculating results and experimental data. The differences in the calculating results for PMS-5 and PMS-50 are explained by differences in the coefficients of surface tension and coefficients of dependence of the surface tension on temperature for these liquids.

Stationary states for different types of silicone oil under the heating power $Q = 16.5$ mW and different initial layer thicknesses are shown in Fig.3. The thickness distributions of PMS-5 and PMS-50 layers with the initial thickness of the silicone oil layer $h_0 = 238$ μm and $h_0 = 538$ μm are shown on Fig. 3 along the cuvette of radius $R_c = 18$ mm. Differences in the calculation results for PMS-5 and PMS-50 are explained by differences in the coefficients of surface tension σ and differences in the coefficient σ_T which determines the dependence of the surface tension on temperature.

PMS-5 has a lower surface tension and, at the same time, depends more on temperature than PMS-50. Both of these contribute to the fact that the deformation for PMS-5 is greater than for PMS-50.

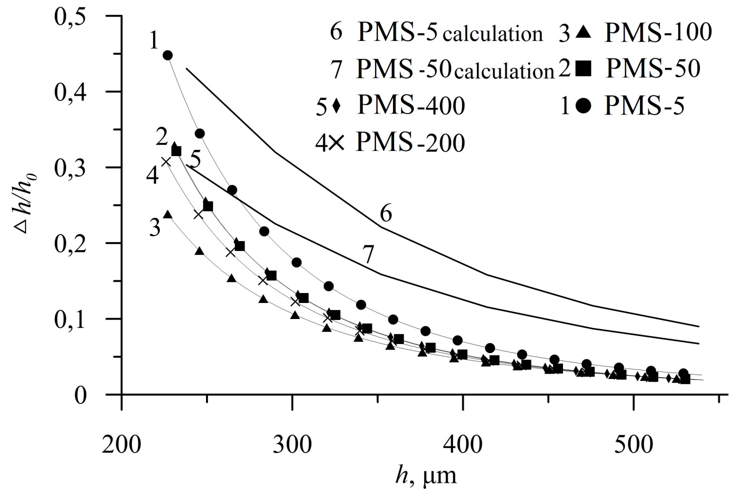

Figure 2: Thermocapillary deformation depth dependence on the thickness of the layer of silicone oil. $\Delta h = h_0 - h_C$ is thermocapillary deformation depth, h_0 is initial thickness of the liquid layer, h_C is layer thickness over the center of the heater at the stage of steady thermocapillary flow. 1 - PMS-5; 2 - PMS-50; 3 - PMS-100; 4 - PMS-200; 5 - PMS-400; 6 - PMS-5 calculations; 7 - PMS-50 calculations.

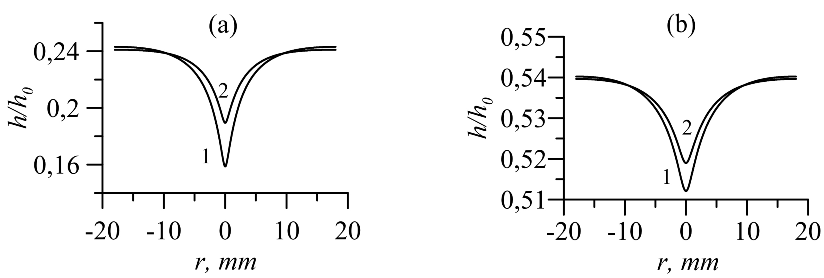

Figure 3: The distribution of the liquid film thickness along the cuvette with radius $R_c = 18mm$ for different types of silicone oil, $t = 100$ s, $Q = 0.0165$ W. 1 - PMS-5; 2 - PMS-50. a) $h_0 = 238$ μm; b) $h_0 = 538$ μm.

The thickness distributions for PMS-5 and PMS-50 along the cuvette of radius R_c at different heating powers, after 2 seconds from the start of heating, are shown on Fig.4. The unsteady state of the process is clearly visible in Fig.4a in the case of PMS-50, where a liquid bump is located at the boundary of the heater, formed due to displacement of the liquid from the center of the cuvette. Since the liquid PMS-50 is more viscous, then within 2 seconds the layer does not have time to spread under the influence of gravity and surface tension. There is a decreasing in the value of the thermocapillary deepening above the heater with increasing thickness of the initial liquid layer, with the same heating of the same liquid.

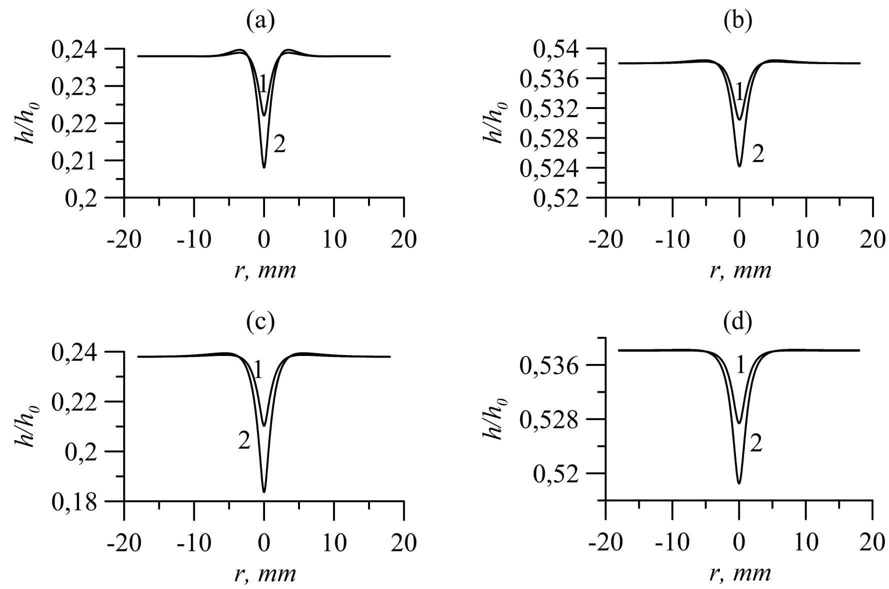

Figure 4: The distribution of the liquid film thickness along the cuvette for different heating values, time $t = 2$s. 1 - $Q = 0.0165$ W; 2 - $Q = 0.3$ W; a) PMS-50, $h_0 = 238$ μm; b) PMS-50, $h_0 = 538$ μm; c) PMS-5, $h_0 = 238$ μm; d) PMS-5, $h_0 = 538$ μm

6 Conclusions

There have been measured and numerically calculated deformations in locally heated horizontal layers of silicone oils of different types and thickness. Numerical calculations have shown that if horizontal liquid layer is locally heated then thermocapillary deformations and thermocapillary flow occurs.

It has been found that the value of the relative deformation of the layer decreases nonlinearly with increasing the layer thickness, when other conditions being equal. The results of modeling using the thin layer approximation are predicting well the main features of the experimental dependences of the thermocapillary deformations on the layer thickness for silicone oils of different types. So the experimental results can be used to test a wide class of computer programs that simulate the processes of heat and mass transfer in multiphase systems with liquid-gas interfaces.

Stationary and unsteady solutions have been obtained for silicone oils of different types. It has been shown that the greater the thickness of the initial layer of silicone oil, the smaller the value of the thermocapillary deepening over the heater with the same heating of the same type of silicone oil.

Dependencies of the depth of thermocapillary deformation on the layer thickness for silicone oils with different viscosities were obtained. It is established that the value of the relative deformation value decreases nonlinearly with increasing initial thickness of the layer. The calculation results are in good qualitative and quantitative agreement with experimental data that had been obtained using confocal microscopy.

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