Numerical modelling of thermocapillary deformation in a locally heated thin horizontal volatile liquid layer

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Abstract. The thermocapillary flow in a thin horizontal layer of viscous incompressible liquid with free surface is considered. The deformable liquid layer is locally heated. The problem of thermocapillary deformation of the locally heated horizontal liquid layer has been solved numerically for two-dimensional unsteady case. The lubrication approximation theory is used. Capillary pressure, viscosity and gravity are taken into account. Evaporating rate is supposed to be proportional to the temperature difference between the liquid surface and ambient. Heat transfer in the substrate is also simulated. The deformation of the free surface has been calculated for different values of the heating power and thickness of the liquid layer. Initially the liquid layer has flat surface and uniform temperature. The model predicts the thermocapillary deformation of the liquid surface and the formation of the thin residual layer of the liquid.

1 Problem statement

Heat transfer in thin liquid layers with local heating is an important challenge for thermal stabilization technique of electronic equipment [1-3]. The problem consider a thin horizontal volatile liquid layer on the substrate with local heater, Figure 1. Liquid is viscous and incompressible. Heater is thin and uniform. Two-dimensional unsteady problem is considered. Initially the liquid layer has flat surface and uniform constant temperature $T_0$. At the time $t_0=0$ the heater is activated and starts heating the substrate and liquid. Shear stress occurs on the liquid surface caused by the heterogeneity of its temperature. Thermocapillary flow and deformation of the liquid layer is developing. The mechanism of convective heat transfer in the liquid and deformation of surface in the heat problem is also taken into account. Gravity, surface tension, thermocapillary effect, viscosity are included in the evolution equation for the liquid layer thickness.

![Figure 1](image_url)

Figure 1. Scheme of the process: liquid layer on the substrate with local heater.
2 Mathematical formulation

2.1 Basic equations

2.1.1 Motion equation of the liquid in the approximation of the lubrication theory

The mathematical formulation of the problem includes the Navier-Stokes equations, continuity and thermal conductivity [4]:

\[
\frac{du}{dt} = F - \frac{1}{\rho} \nabla p + \nu \Delta u
\]

\[
\nabla u = 0
\]

\[
\frac{\partial T}{\partial t} + u \nabla T = a \Delta T + F
\]

(1)

The dimensional variables that are used into equations: \( u \) - velocity, \( F \)- vector of external forces, \( \rho \) - density, \( p \) - capillary pressure, \( \nu \) - kinematic viscosity, \( T \) - temperature, \( a \) - thermal diffusivity.

2.1.2 The evolution equation for liquid film thickness

The evolution equation for liquid film thickness in the case of horizontal substrate, in thin layer approximation [4-6], is as follows:

\[
\frac{dh}{dt} + divq + J_{ev} = 0
\]

(2)

Where, \( h \) - velocity of the surface, \( q = \frac{h^3}{3\mu} f + \frac{h^2}{2\mu} \tau \) - liquid flow rate along the \( x \) direction, \( f = \nabla (\rho gh + \sigma H) \) - gradient of the modified pressure, \( \tau = \sigma_T \nabla T \) - thermocapillary tangent stress, \( \mu \) - dynamic viscosity, \( \rho \) - density of the liquid, \( g \) - gravity vector, \( h \) - film thickness, \( \sigma \) - surface tension, \( \sigma_T \) - linear coefficient, which determines the dependence of the surface tension on temperature, \( T \) - temperature, \( H = h_{xx} \left(1 + h_x^2 \right)^{3/2} \) - double mean curvature.

\( J_{ev} = J_{ev}^* (T_s(x) - T_a) / \Delta T \) - evaporation velocity, \( T_s(x) \) - temperature of the surface, \( J_{ev}^* = \alpha_{ev} / r_h \rho \), \( \alpha_{ev} \) - heat transfer coefficient for evaporation, \( r_h \) - latent heat of vaporization.

2.1.3 The energy equation

The law of temperature distribution in the liquid layer is determined by the energy equation:

\[
\frac{\partial T}{\partial t} + u \nabla T = a \Delta T + \frac{Q}{\rho C_p}
\]

(3)
Where \( Q = Q(t, x, z) = \begin{cases} Q = 0, & \text{outside the heater} \\ Q = \text{const} \neq 0, & \text{on the heater} \end{cases} \) - bulk density of the heat sources, the function \( Q(t, x, z) \) has a constant nonzero value in the area of the heater which is known from the experimental conditions, \( a = \frac{\lambda}{\rho \cdot C_p} \) - thermal diffusivity; \( \lambda \) - coefficient of thermal conductivity; \( C_p \) - specific heat; \( \rho \) - density of the liquid.

### 2.2 The boundary and initial conditions

#### 2.2.1 The boundary conditions

Since it is made the replacement of the variables for the rectification of the liquid surface, then move on to the conjugation conditions at the liquid-substrate interface.

\[
\lambda \frac{\partial T}{\partial z} \bigg|_{z=0} = \alpha_{ev} (T - T_a)
\]

\[
\lambda \frac{\partial T}{\partial x} \bigg|_{x=L} = \alpha (T - T_a), \quad \text{left boundary}
\]

\[
-\lambda \frac{\partial T}{\partial x} \bigg|_{x=0} = \alpha (T - T_a), \quad \text{right boundary}
\]

\[
-\lambda \frac{\partial T}{\partial z} \bigg|_{z=h+h_v} = \alpha (T - T_a), \quad \text{bottom boundary}
\]

\[
\lambda \frac{\partial T}{\partial z} \bigg|_{z=0} = \alpha_{ev} (T - T_a), \quad \text{top boundary}
\]

In the condition of the top boundary \( \alpha_{ev} = J_{ev}^* r_{lv} \rho \), \( \alpha_{ev} \) is the heat transfer coefficient for evaporation, \( r_{lv} \) - latent heat of vaporization, \( J_{ev}^* \) - evaporation rate coefficient. The coefficients for evaporation rates have been calculated using the data published in [7], \( J_{ev}^* = 3.8 \mu \text{m/s} \cdot \text{K} \), \( \alpha_{ev} = 9.72 \text{ kW/m}^2\text{K} \).
2.2.2 The initial conditions

Initially the liquid layer has flat surface and uniform temperature:

\[ h(0, x, z) = h_0 = \text{const}, \quad T(0, x, z) = T_0 = \text{const}. \]

3 Numerical modelling

The evolution equation of the liquid layer thickness (2) is approximated at grid’s nodes with finite volume method [6]. System of nonlinear algebraic equations obtained by the approximation is solved with Newton's method. The Jacobians are calculated using numerical linearization [6]. The grid with uniform steps in the space variables in the liquid and solid phases is set: \( x_i = i \cdot dx, i = 0, ..., N \). The time step \( \tau \) is also uniform. \( h_i^k = h(x_i, t_k) \) is the value of the liquid layer thickness in the time \( t \) and \( i \) node.

\[ \frac{h_i^{k+1} - h_i^k}{\tau} dx^2 + q \frac{1}{2} dx + q \frac{1}{2} dx = 0 \] (5)

Geometric parameters and parameters of the liquid, substrate and heater are specified.

**Table 1**: parameters of the system in 20 °C.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Ethanol, 20 °C</th>
<th>Water, 20 °C</th>
<th>Substrate (sapphire), 20 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho ) density, kg/m³</td>
<td>802.9</td>
<td>998.3</td>
<td>3980</td>
</tr>
<tr>
<td>( C_p ) specific heat, J/kg·m</td>
<td>2390</td>
<td>4182</td>
<td>761</td>
</tr>
<tr>
<td>( \lambda ) coefficient of thermal conductivity, W/m·K</td>
<td>0.1692</td>
<td>0.6092</td>
<td>25</td>
</tr>
<tr>
<td>( \mu ) dynamic viscosity, kg/m·s</td>
<td>0.001145</td>
<td>0.001018</td>
<td></td>
</tr>
<tr>
<td>( r ) latent heat of vaporization, (J/kg)</td>
<td>938200</td>
<td>2563000</td>
<td></td>
</tr>
<tr>
<td>( \sigma ) surface tension, N/m</td>
<td>0.02203</td>
<td>0.07275</td>
<td></td>
</tr>
<tr>
<td>( \sigma_T ) - linear coefficient of the dependence of the surface tension on temperature, (N/m·K)</td>
<td>−0.0000936</td>
<td>−0.0001575</td>
<td></td>
</tr>
</tbody>
</table>

**Heater**

Length \( L_h = 40 \text{mm} \), width \( h_h = 0.5 \text{mm} \), thickness \( h_{\text{heater}} = 0.5 \mu m \), Heating power \( P_h = 3 \text{ W} \)

The temperature in the liquid is calculated without allowance of the deformations, since the heater is thin, it is considered that \( Q = Q(t, r, z) \) is concentrated only in heater units. The difference analog of the energy equation (3) is solved by the method of fractional steps [8].
\[
\frac{T^{n+\frac{1}{2}} - T^n}{\tau} = \frac{1}{2} \left( \Lambda_1 T^{n+\frac{1}{2}} + \Lambda_2 T^n \right) + \frac{Q^n}{2C_p\rho}, \quad \Lambda_1 = \frac{T_{i-1,j} - 2T_{i,j} + T_{i+1,j}}{dx^2}, \\
\frac{T^{n+1} - T^{n+\frac{1}{2}}}{\tau} = \frac{1}{2} \left( \Lambda_1 T^{n+\frac{1}{2}} + \Lambda_2 T^{n+1} \right) + \frac{Q^n}{2C_p\rho}, \quad \Lambda_2 = \frac{T_{i,j-1} - 2T_{i,j} + T_{i,j+1}}{dz^2}
\]

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

\[
T(j,0) = T(j,2), \quad j = 1,..,M, - \text{ symmetry} \\
T(j,N+1) = T(j,N-1), \quad j = 1,..,M - \text{ adiabatic right wall} \\
T(0,i) = T(2,i) - \alpha \lambda (T(1,i) - T_a)2dh, \quad i = 1,..,N \\
T(M+1,i) = T(M-1,i) - \frac{\alpha_w}{\lambda_w} (T(M,i) - T_a)2dh_w, \quad i = 1,..,N
\]

Initial condition: \( T_{i,j}^0 = 0, \quad i = 0,..,N, \quad j = 1,..,M - 1 \).

The resulting system of linear algebraic equations is solved at each step with the tridiagonal matrix algorithm. Calculations are performed successively. The time step for the evolution equation is done after the time step for the energy equation.

## 4 Numerical results

The deformation of the free surface has been calculated for different values of the heating power and thickness of the liquid layer. The model predicts the formation of the thin residual layer of the liquid and film breakdown at sufficiently intensive heating. Calculated deformations of the liquid layer with the time are shown in Fig. 3. The thin residual layer is formed in the center, over the heater. It predicts the formation of dry spots. A local decreasing of the liquid surface temperature is shown in Fig. 4, curve 4. It is caused by the intense evaporation and decreasing of the thermal resistance of the liquid layer.

![Figure 3. Calculated distributions of the liquid layer thickness. 1 – 0.5 s; 2 – 1.0 s; 3 – 1.5 s; 4 – 2.0 s. Heating power 3 W, water.](image-url)
Figure 4. Calculated distributions of the surface temperature. 1 – 0.5 s; 2 – 1.0 s; 3 – 1.5 s; 4 – 2.0 s. Heating power 3 W, water.

Conclusions
The numerical calculations with given model of thin horizontal liquid layer with local heating have shown that local heating of a horizontal liquid layer causes deformation of the liquid surface and thermocapillary flow. Significant reduction of liquid film thickness occurs in the greatest value of the temperature gradient zone. The model predicts the formation of the thin residual layer of the liquid. A local decreasing of the liquid surface temperature is caused by the intense evaporation and the decreasing of the thermal resistance of the liquid layer.

Acknowledgements
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References