Numerical modeling of the liquid film flow with evaporation on the basis of the generalized interface conditions

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Abstract.
A thin layer of a viscous incompressible liquid flowing down an inclined, non-uniformly heated substrate under conditions of a concomitant gas flow is studied. The flow is accompanied by evaporation at the thermocapillary interface. Dynamic processes in a gas are not taken into account (one-side model). The mathematical model of a thin liquid layer flow is based on the Navier-Stokes equation and the heat transfer equation, as well as generalized kinematic, dynamic and energetic conditions at the thermocapillary boundary. The local mass flux at the interface is determined using the Hertz-Knudsen equation. Analytical solutions of the problem are constructed for the zeroth-order terms of the expansions of the desired functions in powers of a small parameter of the problem. Parametric analysis of the problem is performed. An evolutionary equation for determining the thickness of the liquid layer is obtained. An algorithm for numerical solution of the evolutionary equation is constructed. The results of numerical studies of flows of a thin layer of ethanol and HFE-7100 with evaporation at the interface are obtained.

1. Introduction
Evaporation, additional shear stresses and the thermocapillary effect can have a sufficiently strong effect on the nature of the physical process in the case when the liquid flow is accompanied by a gas flow. Therefore, one of the most important points is a formulation of the boundary conditions at the interface [1-4]. A detailed derivation of conditions on the free boundary, which are a consequence of the laws of conservation of mass, momentum, and energy is presented in [5]. Additional hypotheses, the relations of differential geometry, the classical transfer theorem and its surface analogue are used. The boundary conditions taking into account evaporation are derived on the basis of integral conservation laws in [2] using statistical theory and without the assumption of continuity of temperature and tangent velocities, and in [1] under the assumption of a diffusive vapor flow at the interface.

Fluid flows taking into account evaporation are studied in the thin-layer approximation in [6-15]. A two-dimensional long-wave model of an evaporating thin layer of liquid flowing down a nonuniformly heated substrate is considered in [11]. A film of a viscous fluid flowing down on an inclined heated surface is studied in [10] in the three-dimensional case. This problem is solved in a lubrication approximation. Capillarity, gravity and evaporation are taken into account. The
effect of evaporation on finger instability is studied. A detailed description of the problems of modeling the flows of evaporating liquid films and condensible layers, solved in the thin layer approximation, is given in [13]. The velocity of the vapor particles is assumed to be sufficiently small, which makes it possible to consider the vapor as an incompressible liquid.

Thin liquid layer flows taking into account evaporation at the interface are often described by a system of Navier-Stokes equations and heat transfer equation [6, 7]. However, the modeling of such flows can also be carried out on the basis of the classical Oberbeck-Boussinesq equations, i.e. in the case when thermal gravitational convection is taken into account [8, 14]. A comparison of the results of numerical experiments obtained using the Navier-Stokes and Oberbek-Boussinesq equations at various gravity intensities is presented in [14].

2. Mathematical model of the problem
A thin layer of viscous incompressible liquid, flowing down an inclined, non-uniformly heated substrate under conditions of tangential gas flow and evaporation at a thermocapillary interface is studied. The problem is considered in the case when dynamic processes in a gas are not taken into account. However, the shear stresses generated by the gas can be taken into account at the substrate under conditions of tangential gas flow and evaporation at a thermocapillary interface. The solid impermeable substrate is inclined at an angle \( \alpha \) to the horizon. The Ox axis directed along a solid boundary. The position of the interface is determined by the equation \( z = H(x, t) \), and the solid boundary is determined by the equation \( z = 0 \). The gravity vector has the form \( g = (g_1, g_2) = (g \sin \alpha, -g \cos \alpha) \), \( g = |g| \).

Two different length scales are available in the problem of the thin liquid layer flow since the characteristic length of the deformation of the interface substantially exceeds the amplitude of the deformation. Let \( l \) is the longitudinal characteristic length, \( d \) is the transverse characteristic length, and \( l \gg d \). Then \( \varepsilon = d/l \) is a small parameter of the problem. Characteristic longitudinal and transverse velocities \( u_* \) and \( w_* \) are related by the expression: \( w_* = \varepsilon u_* \). Let the characteristic time of the process \( t_* \) related to other parameters of the problem as follows \( t_* = l/u_* \), and the characteristic pressure is set by the expression \( p_* = (\rho u_* \nu l)/d^2 \). Here \( \rho \) is some relative value of liquid density, \( \nu \) is the kinematic viscosity coefficient.

The liquid flow is studied on the basis of a system of Navier—Stokes equations and a heat transfer equation written in the dimensionless form:

\[
Re \varepsilon^2 (u_t + uu_x + wu_z) - \varepsilon^2 u_{xx} = u_{zz} - p_x + \gamma_1 \sin \alpha, \tag{1}
\]
\[
Re \varepsilon^4 (w_t + uw_x + w^2) - \varepsilon^4 w_{xx} - \varepsilon^2 w_{zz} = -p_z - \gamma_2 \cos \alpha, \tag{2}
\]
\[
u_a + w_z = 0, \tag{3}
\]
\[
Re Pr \varepsilon^2 (T_t + u T_x + w T_z) - \varepsilon^2 T_{xx} = T_{zz}. \tag{4}
\]

Here \( v = (u, w) \) is the velocity vector, \( T \) is the temperature, \( p \) is the pressure, \( Pr = \nu/\chi \) is the Prandtl number, \( Re = (u_* l)/\nu \) is the Reynolds number, \( \gamma_1 = Gr/(Bu Re) \), \( \gamma_2 = Gr/(Bu Re) \), \( Gr = (Bu d^3)/\nu^2 \) is the Grashoff number, \( Bu = \beta T_0 \) is the Boussinesq number, \( \chi \) is the thermal diffusivity coefficient, \( \beta \) is the thermal expansion coefficient, \( T_0 \) is the characteristic temperature drop.

The normal vector \( n \) and the tangent vector \( s \) have coordinates \((n_1, n_2)\) and \((n_2, -n_1)\), respectively. Here \( n_1 = -(\varepsilon h_x)/\sqrt{1 + \varepsilon^2 h_x^2}, n_2 = 1/\sqrt{1 + \varepsilon^2 h_x^2} \). The curvature of the free boundary and the velocity of its movement in the direction of the external normal are given by the relations:

\[
2H = \frac{\varepsilon h_{xx}}{\sqrt{1 + \varepsilon^2 h_x^2}}, \quad D_n = -\frac{\varepsilon h_t}{\sqrt{1 + \varepsilon^2 h_x^2}}. \]
The generalized kinematic, dynamic and energetic conditions at the interface $z = h(x,t)$ [3, 4, 8, 16] can be written after simplifications in the following dimensionless form:

$$-\varepsilon(h_t + h_xu - w) = J_{ev}\ddot{f},$$

$$p = p^\theta - \alpha_Ca h_{xx}(1 - \alpha_v T),$$

$$u_z = \alpha_v\tau(x,t) - \alpha_Ma(T_x + h_x T_z),$$

$$-T_z + \beta_2 T_{div} = \beta_3 J_{ev} + \beta_6 u h_{xx} J_{ev}.$$  

The linear dependence of the surface tension coefficient on temperature in a dimensionless form is written as follows:

$$\sigma = 1 - \alpha \sigma T,$$

$$\sigma = (Ma Ca)/(Re Pr).$$

The following designations are introduced: $\alpha_{Ca} = \varepsilon/Ca$, $\alpha_v = \bar{\rho} \bar{v} \varepsilon/\bar{h}$, $\alpha_Ma = Ma \varepsilon/Pr$, $Ma = (T_s T)/(\rho \nu \chi)$ is the Marangoni number, $Ca = (u \nu \chi)/\sigma_0$ is the capillary number, $\bar{v}$, $\bar{p}$ are the ratio of the coefficients of kinematic viscosity and densities of the gas and liquid, respectively, $\bar{v} = u_0^2/u_s$ is the ratio of the characteristic gas velocity to $u_s$; $\bar{h}$ is the ratio of the characteristic scale of gas layer to $l$; $p^\theta$ is the gas pressure. Coefficients $\beta_i$ ($i = 2, 3, 6$) calculated as follows:

$$\beta_2 = (Ma \varepsilon)/(Re^2 Pr E U),$$

$$\beta_3 = (\varepsilon\bar{J})/E,$$

$$\beta_6 = (1 - \bar{\rho})(\varepsilon^2\bar{J})/(Re Ca E U),$$

$$E = (\kappa T_s)/(\lambda_U \rho \nu)$$

is the evaporation coefficient, $\kappa$ is the heat conductivity coefficient, $\lambda_U$ is the latent heat of vaporization. Note that $\bar{J} = J_s^\theta/(\rho u_s)$ or $\bar{J} = E/Re$, where $J_s^\theta$ calculated as follows:

$$J_s^\theta = (\kappa T_s)/(\lambda_U \rho \nu).$$

The local mass flux $J_{ev}$ is determined with the help of the relation (see [11]):

$$J_{ev} = \alpha_J T|_{z=h(x,t)}.$$  

Here coefficient $\alpha_J$ is determined based on Hertz-Knudsen relations [11, 16]: $\alpha_J = \alpha_{p_d} \lambda_U (T_s/J_s)/(M/(2 \pi R_g T_s^3))^{1/2}$, $\alpha$ is the accommodation coefficient, $\rho h_{os}$ is the vapor density, $M$ is the molecular weight, $T_s$ is the saturated vapor temperature, $R_g$ is the universal gas constant.

On the solid boundary $z = 0$ the no-slip conditions and temperature distribution have the form

$$u|_{z=0} = 0, \quad w|_{z=0} = 0;$$

$$T|_{z=0} = \Theta_0(x,t).$$

In the case when the characteristic velocity $u_c$ is equal to the characteristic relaxation rate of viscous stresses $u_v = \nu/l$ the Reynolds number is of order 1 ($Re = O(1)$). Thus, further modeling is applicable for moderate Reynolds numbers.

The system of equations (1)-(4) in the long-wave approximation is considered to determine the sought functions $u, w, T, p$ and the thickness of the liquid layer $h$. The solution of the problem is found in the form of decompositions in powers of the small parameter $\varepsilon$.

The general solutions of functions $u^0, w^0, p^0, T^0$ taking into account the conditions on a solid substrate (6), (7) have the form:

$$u^0 = (C_0) x \frac{z^2}{2} - \gamma_1 \sin \frac{z^2}{2} + C_1 z,$$

$$w^0 = -(C_0) xx \frac{z^3}{6} - (C_1) x \frac{z^2}{2} - (C_2) x,$$

$$p^0 = -\gamma_2 \cos \alpha z + C_0,$$

$$T^0 = A(x,t)z + \Theta_0(x,t).$$
The coefficients $C_0(x, t), C_1(x, t), A(x, t)$ satisfy the following relations:

$$C_0(x, t) = p^0 - \alpha C_0 h_{xx}(1 - \alpha \Theta^0) + \gamma_2 \cos \alpha h, \quad C_1(x, t) = -\alpha_M a \hat{\Theta} - (C_0) h + \gamma_1 \sin \alpha h,$$

$$A = \frac{(-\beta_2(C_1) h + \beta_3 \alpha_j + \beta_4 h_x \alpha_j) \Theta_0}{1 + \beta_2(C_1) h^2 - \beta_3 \alpha_j h - \beta_4 h_x \alpha_j h_x h}.$$

Here $\Theta^0 = Ah + \Theta_0, \hat{\Theta} = A_x h + (\Theta_0)x + h_x A$.

3. The thin layer equation: scheme of the numerical solution

The evolution equation of the film thickness is obtained using the relation (5) and formulas (8),(9):

$$h_t + h_x \left[ \left(C_0(h) \right)_x \frac{h^2}{2} - \gamma_1 \sin \alpha \frac{h^2}{2} + C_1 h \right] + \left(C_0(x) \frac{h^3}{6} + C_1 \frac{h^2}{2} + \frac{E}{\varepsilon} J_{ev} \right) = 0. \quad (13)$$

Here $J_{ev} = \alpha_j [A(x, t)h + \Theta_0(x, t)]$.

The periodic problem of finding a function $h(x, t)$ satisfying the equation (13) on the interval $[-L; L]$ is considered. The following periodic conditions are assumed to be fulfilled:

$$h|_{x=-L} = h|_{x=L}, \quad h_x|_{x=-L} = h_x|_{x=L}, \quad h_{xx}|_{x=-L} = h_{xx}|_{x=L}.$$

Let the initial position of the thermocapillary boundary be determined by the function $h_0(x) = 1 - \delta_0 \cos kx$. The function $\Theta_0$ which determines the non-uniform heating of the substrate (7), is set as follows: $\Theta_0(x, t) = 1 - \delta_1 \cos(k_1 x) \cos(k_2 t)$.

Equation (13) taking into account relations (12) takes the form:

$$h_t + A_1 h_{xxx} + A_2 h_{xx} + A_3 h_{xx} + A_4 h + D = 0. \quad (14)$$

Here the coefficients $A_1, A_2, A_3, A_4, D$ are functions that depend on $A, h, \Theta_0$ and its derivatives.

The implicit finite-difference scheme is used to numerically solve the equation (14):

$$\frac{h^{k+1} - h^k}{\tau} + A_1 k^{k+1}_{xxx} + A_3 k^{k+1}_{xx} + A_2 k^{k+1}_{xx} + A_4 k^{k+1} + D^k = 0. \quad (15)$$

The uniform finite-difference mesh $x_1, x_2, ..., x_{N+1}, x_n = -L + (n - 1)\Delta x, n = 1, 2, ..., N + 1$ with the step $\Delta x = 2L/N$ is introduced to implement an implicit scheme. The finite-difference analogues of the second-order approximation are used for all derivatives with respect to $x$ in (15). The problem reduces to solving a system of linear algebraic equations by the method of five-point sweep and sweep with parameter. The unknown value of the liquid layer thickness $h$ at $x = -L, x = L$ is chosen as the parameter [15].

4. Numerical results

Numerical studies of the process of various liquids films flows are carried out. The figures 1 and 2 show the dynamics of the liquid layer over time in the case of inhomogeneous heating of the substrate. The coefficients that define the initial position of the interface and the heating of the inclined substrate take the following values: $\delta_0 = 0.1, \delta_1 = 0.25, k = k_1 = k_2 = \pi/2$. Ethanol (Fig. 1) and HFE-7100 (Fig. 2) were selected as working liquids. Note that here $\beta_3 = 0.1, \beta_2 = \beta_6 = 0$, i.e. effects that determine the contribution of the energy spent on overcoming the surface deformation by thermocapillary forces along the surface and on the work performed by the liquid substance during evaporation (condensation) due to changes in the specific volume were not taken into account. Thinning of the liquid layer over time is observed for both liquids. The interface is deformed relative to the initial position of the interface (lines —— in the figures 1 and 2). The figures show that in the case when ethanol is chosen as the liquid, the rate of
Figure 1. The behaviour of the liquid layer thickness, the case of choosing ethanol as a liquid: 1 – initial position of the interface; 2 – $t = 10^{-5}$; 3 – $t = 10^{-4}$; 4 – $t = 10^{-3}$.

Figure 2. The behaviour of the liquid layer thickness, the case of choosing HFE-7100 as a liquid: 1 – initial position of the interface; 2 – $t = 10^{-5}$; 3 – $t = 10^{-4}$.

decrease of the liquid layer thickness is lower than in the case of choosing the HFE-7100 (lines $\cdots\cdots$ in the figures 1 and 2).

Figure 3 shows the behavior of the liquid layer in the case when the coefficient $\beta_2^* = 0.3$ (the term determining the contribution of the energy spent on overcoming the surface deformation by thermocapillary forces along the surface is taken into account). The interface is strongly deformed if the term determining the heat consumption for vaporization is taken into account (the line $\cdots\cdots$), and without taking this effect into account (the line $\cdots\cdots\cdots$). Here ethanol is chosen as a liquid.

Figure 3. The behaviour of the liquid layer thickness, the case of choosing ethanol as a liquid, $\beta_2^* = 0.3$: 1 – initial position of the interface; 2 – $\beta_3^* = 0$, $t = 10^{-3}$; 3 – $\beta_3^* = 0.1$, $t = 10^{-3}$. 

5. Conclusion
The mathematical model of thin flow presented in this paper allows us to study the influence of various physical effects such as evaporation, additional tangential stresses, capillary and thermocapillary effects on the nature of the liquid flow. The proposed algorithm of numerical solution makes it possible to determine the thickness of the liquid layer taking into account these effects.

The dependence of the flow character of the liquid layer on the liquid considered in the experiment is numerically studied. It is shown that the thinning of the flowing layer occurs more intensively when the HFE7100 is used as a liquid. The differences between the flow characters in the case when the energy condition is considered in the classical formulation and in the case of a generalized energy condition are considered.

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