Numerical modeling of a thin liquid layer flow on an inclined substrate based on classical convection equations and generalized conditions at the interface

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Abstract. The flow of a thin layer of a viscous incompressible liquid along an inclined non-uniformly heated substrate is investigated in the two-dimensional case. Evaporation is taken into account at the thermocapillary interface. The system of Oberbeck-Boussinesq equations is used as a mathematical model. The kinematic, dynamic and energy conditions generalized for the case of a nonzero mass flux are assumed to be fulfilled at the interface. The value of the local mass flux is determined using the Hertz-Knudsen equation. Solutions to problems for the main terms of power decomposition of a small parameter of the problem are obtained. The evolution equation to determine the position of the interface is obtained. A numerical algorithm for solving the problem is constructed. The problem of periodic runoff of an incompressible liquid layer is considered. The effect of additional terms in the energy condition on the dynamics of the thickness of the liquid layer is studied.

1. Introduction
In the cases of liquid flows accompanied by a gas flow, some effects such as capillary, thermocapillary and gravitation forces, evaporation, additional shear stresses may affect the processes. Therefore, one of the important points in mathematical modelling of joint flows of liquids and gases is the formulation of conditions at the interface. The interface conditions considering the evaporation and integral laws of conservation are derived in [1] under the assumption of a diffusive vapor flux at the interface. In paper [2] these conditions are obtained using statistical theory and without assuming continuity of temperature and tangential velocities. The detailed derivation of the conditions on the free boundary using additional hypotheses, the classical transfer theorem and its surface analogue is given in [3].

In this paper the mathematical model of a viscous incompressible liquid flow is considered based on a long-wave approximation. The system of Oberbeck-Boussinesq equations allows taking into account buoyancy forces in modelling. Kinematic, dynamic, and energetic conditions are generalized for the case of a non-zero vapor flux. The evolution equation that determines the position of the interface and takes into account the effects of evaporation, capillarity and thermocapillarity, viscosity, gravity and additional tangential stresses from the external environment is obtained. The influence of additional effects at the interface on the flow characteristics is demonstrated using numerical results.

2. Problem statement
A thin layer of viscous incompressible liquid flows down on a solid impermeable substrate inclined at an angle $\alpha$ to the horizon line (see figure 1). The coordinate system is introduced so that the Ox axis is...
directed along the solid substrate determined by the equation \( z = 0 \). The position of the interface changes over time and is determined by the equation \( z = h(x,t) \). The gravity vector has the form \( \mathbf{g} = (g_x, g_z) = (g \sin \alpha, -g \cos \alpha) \), where \( g = |\mathbf{g}| \).

**Figure 1.** Geometry of flow domain.

Mathematical modeling is based on the fact that there are two characteristic length scales: longitudinal and transverse. The small parameter of the problem \( \varepsilon \) is the ratio of the transverse length to the longitudinal length (\( \varepsilon = d/l \)).

The Oberbeck-Boussinesq system of equations is used as a one-sided mathematical model of the process. The equations in dimensionless form are as follows:

\[
\begin{align*}
\varepsilon (u_x + uu_x + wu_z) - \varepsilon u_{xx} &= u_{zz} - p_x' - \gamma_1 T \sin \alpha , \\
\varepsilon (w_x + uw_x + w^2) - \varepsilon w_{xx} &= w_{zz} - p_z' + \gamma_2 T \cos \alpha , \\
ux + w_z &= 0 , \\
Pr \varepsilon^2 (T_x + u T_x + w T_z) - \varepsilon^2 T_{xx} &= T_{zz} .
\end{align*}
\]

Here \( \mathbf{v} = (u, w) \) is the velocity vector; \( p \) is the modified pressure \( (p' = p - \gamma_1 (\beta T)^{\frac{1}{2}} x \sin \alpha + \gamma_2 (\beta T)^{\frac{1}{2}} z \cos \alpha) \); \( T \) is the temperature; \( Re = u l / \nu \) is the Reynolds number; \( Pr = \nu / \chi \) is the Prandtl number; \( \gamma_1 = Gr / \varepsilon ; \gamma_2 = Gr; Gr = d^2 g \beta T^2 / \nu^2 \) is the Grasgof number; \( \chi, \nu, \beta \) are the coefficients of the thermal diffusivity, kinematic viscosity and thermal expansion; \( \rho \) is the relative value of the liquid density; \( T_\ast \) is the characteristic temperature drop; and \( u_\ast \) is the characteristic longitudinal velocity of the liquid.

The generalized kinematic, dynamic and energetic conditions [4, 5] in a dimensionless form after simplification are written as follows:

\[
- \varepsilon (h_z + h u_z - w) = E J_{ev} ,
\]

\[
u_z = \alpha_e \tau (x,t) - \alpha_{Ma} (T_x + h T_z) ,
\]

\[
p = p' - \alpha_{Ca} h_x (1 - \alpha) T ,
\]

\[
- T_\ast + \beta T \nu_{div} \nu = \beta_3 J_{ev} + \beta_6 h_x J_{ev} .
\]

Here \( E = \kappa T / (\alpha U \rho \nu) \) is the evaporation parameter, \( J_{ev} \) is the local mass flux at the thermocapillary interface, \( \alpha_e = \rho \nu \kappa / l \), \( \alpha_{Ma} = Ma / Pr \), \( \alpha_{Ca} = \nu / Ca \), \( \alpha_{Ma} = Ma Ca / Pr \); \( \beta_3 = (MaCa / (Re^2 Pr E \bar{U})) \) are the dimensionless coefficients in the term, which determine the contribution of the energy spent on overcoming the surface deformation by thermocapillary forces along the surface, \( \beta_3 = (\varepsilon J / E) \) is the dimensionless coefficient in the term, which determines the heat consumption for vaporization, \( \beta_6 = (1 - 1 / \rho) (\varepsilon^2 / J) / (Re \bar{Ca} E \bar{U}) \) is the dimensionless coefficient in the term, which determines the contribution of the energy spent on the work performed by the liquid substance during evaporation (condensation) due to changes in the specific volume, \( \kappa \) is the heat conductivity coefficient, \( \lambda_{UV} \) is the latent heat of vaporization, \( \bar{\rho}, \bar{\nu} \) are the ratios of the density and the coefficient of kinematic viscosity of the gas and liquid, \( \bar{\lambda} \) is the ratio of the characteristic scale of gas layer to \( l \), \( Ma = \sigma T l / (\rho \nu \gamma) \) is the Marangoni number, and \( Ca = \nu \rho \nu / \sigma \bar{b} \bar{s} \) is the capillary number, \( \bar{U} = \lambda_{UV} / u_z^2 \). The
surface tension is assumed to be linearly dependent on temperature: \( \sigma = \sigma_0 + \sigma_f (T - T_0) \). Here \( \sigma_0 \) is the value of the coefficient of surface tension \( \sigma \) at some temperature value, \( \sigma_f \) is the temperature coefficient of surface tension.

The local vapor mass flux at the interface \( J_{ev} \) is determined with help of the Hertz-Knudsen equation [6, 7]: \( J_{ev} = \alpha \rho_x T \), where \( \alpha \rho_x T \) is the accommodated flux per unit area, \( \alpha \) is the accommodation coefficient \( J \)-is the characteristic value of the vapor mass flux, \( \rho_x \) is the vapor density, \( T \) is the saturated vapor temperature, \( M \) is the molecular weight, \( R \) is the universal gas constant.

The no-slip conditions for the longitudinal and transverse velocities are given on the solid plate:

\[
u_{\parallel=0} = 0, \quad v_{\perp=0} = 0.
\]

The problem statement is also supplemented with initial conditions.

3. The thin liquid layer equation: numerical solution

The problem is considered in the long-wave approximation. The solution of the unknown functions (longitudinal and transverse velocities, temperature and pressure) is found in the form of a power expansion of a small parameter of the problem \( \varepsilon \). The problem of finding the unknown functions will be solved after obtaining the liquid layer thickness \( h \). In this paper we consider the problem statement for the zero-th order terms of the expansion in powers of \( \varepsilon \) of the unknown functions. The evolution equation takes place to determine the liquid layer thickness (a consequence of the kinematic condition (1)) [8, 9]:

\[
h + h
\left[\frac{h}{2} \gamma_2 \cos \alpha A + \frac{h^3}{6} \left( \gamma_2 \cos \alpha (\Theta_0) + \gamma_1 \sin \alpha A \right) + \frac{h^2}{2} \left( \left( \Theta_0 \right) + \gamma_1 \sin \alpha \Theta_0 \right) + C h \right] +
\]

\[
+ \left[ \frac{h^5}{120} \gamma_2 \cos \alpha A + \frac{h^5}{24} \left( \gamma_2 \cos \alpha (\Theta_0) + \gamma_1 sin \alpha A \right) + \frac{h^3}{6} \left( \left( \Theta_0 \right) + \gamma_1 \sin \alpha \Theta_0 \right) + \frac{h^2}{2} \left( \Theta_0 \right) \right] + (2)
\]

Here functions \( A, C_0, C_1 \) and \( C_2 \) can be found from the following formulas:

\[
A = \frac{\left( -\beta_2 \left( \Theta_0 \right) + h + \beta_1 \alpha \right)}{1 + \beta_1 \left( \Theta_0 \right) + h - \beta_0 \alpha,} \quad \Theta_0\]

\[
C_0 (x, t) = p - \alpha_c h \left( \left( \Theta_0 \right) + \gamma_2 \cos \alpha \right) \quad C_1 (x, t) = \alpha_{\Theta} \left( \Theta_0 \right) + \gamma_2 \cos \alpha \]

The function \( \Theta_0 \) defines the temperature distribution on the solid substrate, \( \Theta_0 = A h + (\Theta_0 \alpha) + h \alpha A \), \( \Theta_0 = \Theta_0 \).

The periodic problem of finding the liquid layer thickness is considered in the interval \([-L; L]\). The following periodic conditions on the boundaries \( x=-L, x=L \) are fulfilled:

\[
h \left|_{x=L} = h \left|_{x=-L}, \quad h \left|_{x=L} = h \left|_{x=-L}, \quad h \left|_{x=L} = h \left|_{x=-L} \right. \right. \right. \right. \]

Equation (2) is solved numerically by using the implicit finite-difference scheme of the following form [8, 9]:

\[
\frac{h_{x+1} - h}{\tau} + A_1 h_{x+1} + A_2 h_{x+1} + A_3 h_{x+1} + A_4 h_{x+1} + A_5 h_{x+1} + D_5 = 0
\]

(3)

Here \( A_4, A_3, A_2, A_1, D \) are the coefficients which depend on \( A, h, \Theta_0 \) and their derivatives. All derivatives with respect to the dimensional variable \( x \) in scheme (3) are approximated using second-order finite-difference analogs. The uniform finite-difference mesh \( x_1, x_2, \ldots, x_{N+1} \) is used for implementation of the scheme (3). Here \( x_0 = -L + (n-1) \Delta x, \Delta x = 2L/N \). The numerical scheme is reduced to a system of linear algebraic equations of the form

\[
b_{x+1} h_{x+1} + c_{x+1} h_{x+1} + d_{x+1} h_{x+1} = d_{x+1}.
\]
\[ a_n^k h_{n-2}^k + b_n^k h_{n-1}^k + c_n^k h_n^k + e_n^k h_{n+1}^k + f_n^k h_{n+2}^k = d_n^k, \quad n = 3, 4, \ldots, N - 1; \]
\[ a_N^k h_{N-2}^k + b_N^k h_{N-1}^k + c_N^k h_N^k + e_N^k h_{N+1}^k + f_N^k h_{N+2}^k = d_N^k. \]  

The system (4) can be solved by using the five-point sweep method and the parametric sweep method. The unknown value of the thickness of the liquid layer \( h \) at \( x = -L, x = L \) is chosen as the parameter.

4. Numerical results
The periodic runoff of a liquid layer on a uniformly heated substrate (\( \Theta_0 = 1 \)) is numerically studied. Physicochemical parameters of ethanol are used as input parameters of the problem. The position of the interface at the initial time is determined by the relation \( h_0(x) = 1 - \delta_0 \cos(kx) \). Here \( k = \pi/2, \delta_0 = 0.01, \) and \( L = 2. \)

Figure 2 shows the dependence of the interface position on additional terms in the energy condition at dimensionless time \( t = 10^{-3} \). Solid substrate is inclined at an angle \( \pi/8 \). The position of the interface is slightly deformed when the energy condition is considered in the classical formulation. In the case of taking into account the term determining the energy consumption for overcoming the surface deformation by thermocapillary forces along the surface, the interface is deformed more strongly than in the previous case. The largest amplitude of changes in the liquid layer thickness in the studied segment is observed in the case of taking into account the term determining the heat consumption for the work performed by the liquid during evaporation (condensation) due to changes in the specific volume.

![Figure 2. Influence of additional terms in the energy condition on the thickness of the liquid layer, \( t = 10^{-3} \).](image)

1. \( \beta_3 = 0.1, \beta_2 = \beta_0 = 0; \)
2. \( \beta_3 = 0.1, \beta_2 = 0.3, \beta_0 = 0; \)
3. \( \beta_3 = 0.1, \beta_2 = 0.3, \beta_0 = -1.2. \)

Conclusions
A mathematical model of the flow of a thin liquid layer along an inclined substrate has been constructed, taking into account evaporation, capillary, thermocapillary and gravitational forces, and additional tangential stresses of the ambient medium. An evolutionary equation defining the position of the interface has been obtained. An numerical solution algorithm has been constructed. The influence of additional terms in the energy condition (the term, which determines the contribution of the energy spent on overcoming the surface deformation by thermocapillary forces along the surface and the term, which determines the contribution of the energy spent on the work performed by the
liquid substance during evaporation (condensation) due to changes in the specific volume) at the interface on the qualitative picture of the flow has been revealed.

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