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HYDROGASDYNAMICS IN TECHNOLOGICAL PROCESSES

HEAT AND MASS EXCHANGE IN FILMS OF A REACTING MIXTURE AND A COOLING LIQUID UNDER EXOTHERMIC-REACTION CONDITIONS

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Conjugate turbulent heat and mass exchange in fast exothermic reactions in thin films has been investigated with allowance for the change in the pressure. A modification of the equal-flow-rate method, the most natural for problems of such a kind, has been constructed. Its distinctive feature is that it is constructed on formal passage to a rectangular domain of variation in variables. The modification obtained has been tested on the problem solved earlier by the well-known equal-flow-rate method. Despite the fact that the proposed mathematical model and the procedure of its investigation enjoy rather wide application, in the present work, it is oriented toward the cationic liquid-phase polymerization of isobutylene. The local concentration distributions of the monomer and the catalyst and the temperature distributions have been obtained in numerical investigations. The reaction and cooling zones have been singled out; it has been recorded that the process of the most active chemical transformation is localized by the narrow zone of entry into the film.

Introduction. Growing interest in nanotechnologies, enabling us, among other things, to directly control the process of production of new materials at a nanoscale level inaccessible before, makes us use another approach to many chemical-engineering processes that are based on a complex set of transformations in multicomponent multiphase systems.

In this connection, film-type flow reactors (initially based on the principle of organization of reaction processes in a thin film of a substance, particularly in the turbulent flow regime where the structure of the free surface of a liquid film has a nanoscale) deserve special attention for liquid-gas-phase processes. The development of such reactors is accompanied by solution of numerous difficult fundamental chemical-engineering problems belonging to both the chemistry and physics of transformations and the nonlinear fields of hydrodynamics and heat and mass transfer in multicomponent multiphase processes [1].

Below, we investigate a mathematical model of a film-type flow reactor in which thin films of a reacting liquid and of that cooling it freely flow, under gravity, down a vertical wall separating them. Selection of the parametric region in the numerical investigation carried out is oriented toward fast highly exothermic transformation processes, such as cationic liquid-phase polymerization of isobutylene [2].

Formulation of the Problem. Consideration is given to a two-dimensional model of two films of liquids freely flowing down, under gravity and at atmospheric pressure, on both sides of a thin (negligible) heat-conducting barrier. One film is a reacting mixture, and the other is cooling water.

Let us direct the Ox axis along the motion of the films (collinearly to the gravity action) and the Oy axis orthogonally to the barrier separating the films. According to [2], the distributions of the components as a consequence of the reaction in a moving mixture film, in the reactor of length L, can be described by the equations

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$$\frac{\partial C_{\mathrm{a}}}{\partial t} + W_1 \frac{\partial C_{\mathrm{a}}}{\partial x} + W_2 \frac{\partial C_{\mathrm{a}}}{\partial y} = \mathrm{div}\,(D_{\mathrm{a}}\,\mathrm{grad}\,(C_{\mathrm{a}})) - K_{\mathrm{a}} C_{\mathrm{a}} C_{\mathrm{b}} \exp\left(-\frac{E_{\mathrm{a}}}{RT_{\mathrm{c}}}\right), \tag{1}$$

$$\frac{\partial C_{\mathrm{b}}}{\partial t} + W_1 \frac{\partial C_{\mathrm{b}}}{\partial x} + W_2 \frac{\partial C_{\mathrm{b}}}{\partial y} = \mathrm{div}\,(D_{\mathrm{b}}\,\mathrm{grad}\,(C_{\mathrm{b}})) - K_{\mathrm{b}} C_{\mathrm{b}} \exp\left(-\frac{E_{\mathrm{b}}}{RT_{\mathrm{c}}}\right), \quad 0 \le x \le L\,, \quad 0 \le y\,. \tag{2}$$

The thermal regime in the film of the reacting mixture is described with allowance for the thermal effect due to the transformations in it and for the motion of the film. It is believed that the heat capacities and thermal conductivities of both the reacting mixture and the water cooling it undergo no substantial changes in all stages of the process:

$$c_{\mathrm{c}}\rho_{\mathrm{c}}\left(\frac{\partial T_{\mathrm{c}}}{\partial t} + W_1 \frac{\partial T_{\mathrm{c}}}{\partial x} + W_2 \frac{\partial T_{\mathrm{c}}}{\partial y}\right) = \mathrm{div}\,(\lambda_{\mathrm{c}}\,\mathrm{grad}\,(T_{\mathrm{c}})) + Q_{\mathrm{c}} K_{\mathrm{a}} C_{\mathrm{a}} C_{\mathrm{b}} \exp\left(-\frac{E_{\mathrm{a}}}{RT_{\mathrm{c}}}\right), \quad 0 \le x \le L\,, \quad 0 \le y\,; \tag{3}$$

$$c_{\mathrm{w}}\rho_{\mathrm{w}}\left(\frac{\partial T_{\mathrm{w}}}{\partial t} + V_1 \frac{\partial T_{\mathrm{w}}}{\partial x} + V_2 \frac{\partial T_{\mathrm{w}}}{\partial y}\right) = \mathrm{div}\,(\lambda_{\mathrm{w}}\,\mathrm{grad}\,(T_{\mathrm{w}}))\,, \quad 0 \le x \le L\,, \quad y \le 0\,. \tag{4}$$

At the boundary $y = 0$ (barrier down which the film flow), we select conjugation conditions (3) and (4) in the form of the equality of the temperatures and temperature fluxes

$$T_{\mathrm{w}}\,(\breve{t}, \breve{x}, 0) = T_{\mathrm{c}}\,(\breve{t}, \breve{x}, 0)\,, \quad \lambda_{\mathrm{w}} \frac{\partial T_{\mathrm{w}}}{\partial \breve{y}}\,(\breve{t}, \breve{x}, 0) = \lambda_{\mathrm{c}} \frac{\partial T_{\mathrm{c}}}{\partial \breve{y}}\,(\breve{t}, \breve{x}, 0)\,. \tag{5}$$

Formulas (5) characterize the conjugation and adhesion conditions.

Next, it is assumed that the total density of the mixture, which includes the starting components and the catalyst and the intermediate and end product, remains constant throughout the process; furthermore, the mixture is assumed to be incompressible. An analogous assumptions is made for the cooling water film, which is in good agreement with experimental data [1].

For analysis of the fundamental pattern of operation of a film-type reactor the case of the stationary (steady-state) motion of films is of prime interest (this case is considered in the present work). This motion is described within the framework of the general approach presented in [1]:

for the reacting mixture

$$\mathrm{div}\,(\mathbf{W}) = 0\,, \quad \mathbf{W}\cdot\mathrm{grad}\,(W_1) = -\frac{1}{\rho_{\mathrm{c}}}\frac{\partial p}{\partial \breve{x}} + \mathrm{div}\left(\left(\sigma_{\mathrm{c}}^{\mathrm{kin}} + \sigma_{\mathrm{c}}^{\mathrm{turb}}\right)\mathrm{grad}\,(W_1)\right) + g\,,$$

$$\mathbf{W}\cdot\mathrm{grad}\,(W_2) = -\frac{1}{\rho_{\mathrm{c}}}\frac{\partial p}{\partial \breve{y}} + \mathrm{div}\left(\left(\sigma_{\mathrm{c}}^{\mathrm{kin}} + \sigma_{\mathrm{c}}^{\mathrm{turb}}\right)\mathrm{grad}\,(W_2)\right), \tag{6}$$

$$\int\limits_0^{k_{\mathrm{c}}(\breve{x})} W_1\,(\breve{x}, s)\,ds = S_{\mathrm{c}} \overset{\mathrm{def}}{\equiv} \int\limits_0^{h_{\mathrm{c}}(0)} W_1\,(0, s)\,ds\,, \quad 0 \le \breve{x} \le L\,, \quad 0 \le \breve{y} \le h_{\mathrm{c}}\,(x)\,;$$

for the aqueous film

$$\mathrm{div}\,(\mathbf{V}) = 0\,, \quad \mathbf{V}\cdot\mathrm{grad}\,(V_1) = -\frac{1}{\rho_{\mathrm{c}}}\frac{\partial p}{\partial \breve{x}} + \mathrm{div}\left(\left(\sigma_{\mathrm{w}}^{\mathrm{kin}} + \sigma_{\mathrm{w}}^{\mathrm{turb}}\right)\mathrm{grad}\,(V_1)\right) + g\,,$$

$$\mathbf{V}\cdot\mathrm{grad}\,(V_2) = -\frac{1}{\rho_c}\frac{\partial p}{\partial \breve{y}} + \mathrm{div}\left(\left(\sigma_{\mathrm{w}}^{\mathrm{kin}} + \sigma_{\mathrm{w}}^{\mathrm{turb}}\right)\mathrm{grad}\,(V_2)\right), \tag{7}$$

$$\int\limits_{h_{\mathrm{w}}(\breve{x})}^{0} V_1\,(\breve{x}, s)\,ds = S_{\mathrm{w}} \overset{\mathrm{def}}{\equiv} \int\limits_{h_{\mathrm{w}}(0)}^{0} V_1\,(0, s)\,ds\,, \quad 0 \le \breve{x} \le L\,, \quad h_{\mathrm{w}}\,(\breve{x}) \le \breve{y} \le 0\,.$$

Here the function $\breve{y} = h(\breve{x})$ with a corresponding subscript describes the free film surface, and the *a priori* known quantity S (called the *flow rate*) remains constant within the framework of the stationary process by virtue of the assumptions made above. Also, it is assumed that the gas contacting the free surface of the reacting-mixture film exerts no pronounced influence on the transformation processes in it [2].

According to experimental data [2], the influence of heat release of the chemical nature under the conditions of stationary motion of films on the character of their motion can be disregarded. In so doing, we can consider the hydrodynamic part of the mathematical model of a film-type reactor irrespective of its thermochemical part. At the same time, an analysis of this part cannot be made in total isolation from the hydrodynamic aspects. All this has determined the numerical analysis of this model in two steps: in the first step, we investigated the hydrodynamics of the flow-type reactor, in the second, we studied chemical transformations under the conditions of the precomputed hydrodynamic pattern. Moreover, this approach has enabled us to test a new modification of the equal-flow-rate method, specially constructed for simultaneous treatment of both problems, which we plan to carry out in subsequent investigations.

Hydrodynamic Part of the Model. The aforesaid and the fact that the film flows in one direction on both sides of the fixed diffusion-impermeable (but heat-conducting) wall enables us to reduce the model's hydrodynamic part to solution of one and the same system of equations but with different values of the parameters.

The system of equations thus obtained is classical for film flow theory and has been investigated, together with its numerous modifications, in [1]. However, this work did not seek to coordinate (much less to simultaneously perform) hydrodynamic calculations with a two-dimensional numerical analysis of exothermic chemical transformations in moving films. Among the difficulties arising in this path, of particular importance is the spatial domain which is occupied by the reacting film and is the integration domain of the thermochemical problem. The most optimum for the latter is the variable-direction method whose application requires a rectangular domain of determination of variables. This section is devoted to overcoming this obstacle by passage to the corresponding new variables.

The hydrodynamics of stationary film flow of the reacting mixture and water can formally be described using the system

$$\mathrm{div}\,(\mathbf{U}) = 0\,, \quad \mathbf{V}\cdot\mathrm{grad}\,(U_1) = -\frac{1}{\rho_c}\frac{\partial p}{\partial \breve{x}} + \mathrm{div}\left(\left(\sigma_{\mathrm{w}}^{\mathrm{kin}} + \sigma_{\mathrm{w}}^{\mathrm{turb}}\right)\mathrm{grad}\,(U_1)\right) + g\,,$$

$$\mathbf{V}\cdot\mathrm{grad}\,(U_2) = -\frac{1}{\rho_c}\frac{\partial p}{\partial \breve{y}} + \mathrm{div}\left(\left(\sigma_{\mathrm{w}}^{\mathrm{kin}} + \sigma_{\mathrm{w}}^{\mathrm{turb}}\right)\mathrm{grad}\,(U_2)\right), \tag{8}$$

$$\int\limits_{0}^{h(\breve{x})} U_1\,(\breve{x}, s)\,ds = S \overset{\mathrm{def}}{\equiv} \int\limits_{0}^{h_0} U_1\,(0, s)\,ds\,, \quad 0 \le \breve{x} \le L\,, \quad 0 \le \breve{y} \le h\,(\breve{x})\,.$$

The character of representation of viscosity as the sum of two components — kinetic and turbulent ones — is selected in accordance with [1] (where the argument and corresponding references have been given):

$$\sigma^{\mathrm{kin}} = \sigma_0 \equiv \mathrm{const}\,, \quad \sigma^{\mathrm{turb}} = \sigma_1\left(1 - \left(\frac{2\breve{y}}{h\,(\breve{x})} - 1\right)^2\right), \tag{9}$$

The right-hand side of (9) points to the most natural substitution of coordinates which reduces the domain of functions of the system transformed to a rectangle. Let us represent the unknown function $h(x)$ as $h(x) = h_0 \exp\,(v(x/\Delta x))$, where Δx is a certain scale of $\breve{x}$ which will be determined below. Then the selected substitution of coordinates can be written in the form

$$\left.\begin{aligned} x &= \frac{\breve{x}}{\Delta x} \\ y &= 2\,\frac{\breve{y}}{h\,(\tilde{x})} - 1 \end{aligned}\right\} \Rightarrow \left.\begin{aligned} \frac{\partial}{\partial \tilde{x}} &= \frac{1}{\Delta x}\left(\frac{\partial}{\partial x} - (1+y)\,\frac{\partial v}{\partial x}\,\frac{\partial}{\partial y}\right) \\ \frac{\partial}{\partial \tilde{y}} &= \frac{2}{h_0 \exp\,(v\,(x))}\,\frac{\partial}{\partial y} \end{aligned}\right\} . \tag{10}$$

This substitution corresponds to the expression of the new velocity vector $\mathbf{w} = (w_1,\ w_2)$ by the previous $\mathbf{U}$:

$$\left.\begin{aligned} w_1 &= \frac{U_1}{\Delta x} \\ w_2 &= -\,2\,\frac{\breve{y}}{h^2}\,\frac{dh}{d\breve{x}}\,U_1 + 2\,\frac{1}{h}\,U_2 \end{aligned}\right\} \Leftrightarrow \left.\begin{aligned} U_1 &= w_1\,\Delta x \\ U_2 &= \left(\frac{(1+y)}{2}\,\frac{dv}{dx}\,w_1 + \frac{1}{2}\,w_2\right) h_0 \exp\,(v\,(x)) \end{aligned}\right\} . \tag{11}$$

In addition to this substitution of variables, we carry out the substitution of unknowns $\mathbf{w} = (w_1,\ w_2)$:

$$\left.\begin{aligned} w_1 &= \exp\,(-\,v\,(x))\,u_1 \\ w_2 &= \exp\,(-\,v\,(x))\,u_2 \end{aligned}\right\} \Rightarrow \left.\begin{aligned} U_1 &= \Delta x \exp\,(-\,v\,(x))\,u_1 \\ U_2 &= \left(\frac{(1+y)}{2}\,\frac{dv}{dx}\,u_1 + \frac{1}{2}\,u_2\right) h_0 \end{aligned}\right\} . \tag{12}$$

It is noteworthy that, on the substitution of variables (10), equality (9) takes the form

$$\sigma_{\mathrm{c}}^{\mathrm{kin}} + \sigma_{\mathrm{c}}^{\mathrm{turb}} = -\,\sigma_1 y^2 + \sigma_1 + \sigma_0 = \sigma_0\,(-\,\sigma y^2 + \sigma + 1)\,. \tag{13}$$

Substituting the right-hand sides of (10) and (12) into the first equation of (8), we obtain

$$\operatorname{div}\,(\mathbf{u}) = 0\,. \tag{14}$$

The second equation of (8) in new variables acquires the form

$$\begin{aligned} &\left(u_1\,\frac{\partial u_1}{\partial x} + u_2\,\frac{\partial u_1}{\partial y} - u_1^2\,\frac{\partial v}{\partial x}\right)\exp\,(-\,2v) = -\,\frac{1}{\rho\,(\Delta x)^2}\,\frac{\partial p}{\partial x} + \frac{y+1}{\rho\,(\Delta x)^2}\,\frac{dv}{dx}\,\frac{\partial p}{\partial y} + \frac{g}{\Delta x} \\ &+ \frac{\sigma_0\,(1+\sigma-\sigma y^2)}{(\Delta x)^2}\exp\,(-\,v)\,\frac{\partial^2 u_1}{\partial x^2} - \frac{2\sigma_0\,(1+\sigma-\sigma y^2)}{(\Delta x)^2}\exp\,(-\,v)\,(1+y)\,\frac{dv}{dx}\,\frac{\partial^2 u_1}{\partial y \partial x} \\ &+ \frac{\sigma_0\,(1+\sigma-\sigma y^2)}{h_0^2}\exp\,(-\,v)\left(\frac{h_0^2\,(1+y)^2}{(\Delta x)^2}\left(\frac{dv}{dx}\right)^2 + \frac{4}{\exp\,(2v)}\right)\frac{\partial^2 u_1}{\partial y^2} \\ &- \frac{2\sigma_0\,(1+\sigma-\sigma y-2\sigma y^2)}{(\Delta x)^2}\,\frac{dv}{dx}\exp\,(-\,v)\,\frac{\partial u_1}{\partial x} + \frac{\sigma_0}{h_0^2}\exp\,(-\,v)\left[\frac{h_0^2}{(\Delta x)^2}\left[(1+y)\,(3+3\sigma-2\sigma y-5\sigma y^2)\left(\frac{dv}{dx}\right)^2\right.\right. \\ &\left.\left. -\,(1+y)\,(1+\sigma-\sigma y^2)\,\frac{d^2 v}{dx^2}\right] - \frac{8\sigma y}{\exp\,(2v)}\right]\frac{\partial u_1}{\partial y} + \frac{\sigma_0}{(\Delta x)^2}\exp\,(-\,v) \end{aligned}$$

$$\times \left[(1 + \sigma - 2\sigma y - 3\sigma y^2) \left(\frac{dv}{dx} \right)^2 + (1 + \sigma - \sigma y^2) \frac{d^2 v}{dx^2} \right] u_1 \, . \tag{15}$$

The third equation of (8) in new variables takes the form

$$\begin{aligned}
&\frac{\exp(-v)}{2} \left[(1 + y) \frac{dv}{dx} \left(u_1 \frac{\partial u_1}{\partial x} + u_2 \frac{\partial u_1}{\partial y} \right) + u_1 \frac{\partial u_2}{\partial x} + u_2 \frac{\partial u_2}{\partial y} + (1 + y) \frac{d^2 v}{dx^2} u_1^2 + u_1 u_2 \frac{dv}{dx} \right] \\
&= \frac{2}{\rho h_0^2 \exp(v)} \frac{\partial p}{\partial y} + \frac{\sigma_0 (1 + \sigma - \sigma y^2)(1 + y)}{2 (\Delta x)^2} \frac{dv}{dx} \frac{\partial^2 u_1}{\partial x^2} - \frac{\sigma_0 (1 + \sigma - \sigma y^2)(1 + y)^2}{(\Delta x)^2} \left(\frac{dv}{dx} \right)^2 \frac{\partial^2 u_1}{\partial y \partial x} \\
&+ \frac{\sigma_0 (1 + \sigma - \sigma y^2)(1 + y)}{2 h_0^2} \left[\frac{h_0^2}{(\Delta x)^2} \left(\frac{dv}{dx} (1 + y) \right)^2 + \frac{4}{\exp(2v)} \right] \frac{dv}{dx} \frac{\partial^2 u_1}{\partial y^2} + \frac{\sigma_0 (1 + \sigma - \sigma y^2)}{2 (\Delta x)^2} \frac{\partial^2 u_2}{\partial x^2} \\
&- \frac{\sigma_0 (1 + \sigma - \sigma y^2)}{(\Delta x)^2} (1 + y) \frac{dv}{dx} \frac{\partial^2 u_2}{\partial y \partial x} + \frac{\sigma_0 (1 + \sigma - \sigma y^2)}{2 h_0^2} \left[\frac{h_0^2}{(\Delta x)^2} \left(\frac{dv}{dx} (1 + y) \right)^2 + \frac{4}{\exp(2v)} \right] \frac{\partial^2 u_2}{\partial y^2} \\
&+ \frac{\sigma_0}{(\Delta x)^2} (1 + y) \left[\frac{d^2 v}{dx^2} (1 + \sigma - \sigma y^2) - \left(\frac{dv}{dx} \right)^2 (1 + \sigma - \sigma y - 2\sigma y^2) \right] \frac{\partial u_1}{\partial x} \\
&+ \frac{\sigma_0}{2 h_0^2} \Bigg[\frac{h_0^2}{(\Delta x)^2} \Bigg[\left(\frac{dv}{dx} \right)^2 (1 + y)^2 (3 + 3\sigma - 2\sigma y - 5\sigma y^2) - 3 \frac{d^2 v}{dx^2} (1 + y)^2 (1 + \sigma - \sigma y)^2 \Bigg] \\
&+ \frac{8}{\exp(2v)} (1 + \sigma - \sigma y - 2\sigma y^2) \Bigg] \frac{dv}{dx} \frac{\partial u_1}{\partial y} + \frac{\sigma_0}{(\Delta x)^2} \sigma y (1 + y) \frac{dv}{dx} \frac{\partial u_2}{\partial x} \\
&- \frac{\sigma_0}{2 (\Delta x)^2} \left[\frac{d^2 v}{dx^2} (1 + y)(1 + \sigma - \sigma y^2) - \left(\frac{dv}{dx} \right)^2 (1 + y)(1 + \sigma - 2\sigma y - 3\sigma y^2) + \frac{8 (\Delta x)^2 \sigma y}{h_0^2} \right] \frac{\partial u_2}{\partial y} \\
&+ \frac{\sigma_0}{2 (\Delta x)^2} \Bigg[\frac{d^3 v}{dx^3} (1 + y)(1 + \sigma - \sigma y^2) + \left(\frac{dv}{dx} \right)^3 (1 + y)(1 + \sigma - 2\sigma y - 3\sigma y^2) \\
&- \left(\frac{dv}{dx} \right)^2 \frac{dv}{dx} (1 + y)(3 + 3\sigma - 2\sigma y - 5\sigma y^2) + \frac{8 (\Delta x)^2 y \sigma}{h_0^2 \exp(2v)} \frac{dv}{dx} \Bigg] u_1 \, .
\end{aligned} \tag{16}$$

Turbulent film flow is known to classically be [3] described within the framework of the Prandtl approximation of Navier–Stokes equations (second and third equations in system (8)). For Eqs. (15) and (16) we also use an analog of this procedure by recognizing that Δx is selected orders of magnitude larger than the initial film thickness h_0; therefore, it may be considered that

$$\frac{h_0^2}{(\Delta x)^2} \approx 0 \, . \tag{17}$$

With account for (17), the asymptotic approximation of (15) will have the form

$$\left(u_1 \frac{\partial u_1}{\partial x} + u_2 \frac{\partial u_1}{\partial y} - u_1^2 \frac{\partial v}{\partial x}\right) \exp(-2v) = -\frac{1}{\rho\,(\Delta x)^2} \frac{\partial p}{\partial x} + \frac{y+1}{\rho\,(\Delta x)^2} \frac{dv}{dx} \frac{\partial p}{\partial y} + \frac{g}{\Delta x}$$

$$+ \frac{\sigma_0\,(1+\sigma-\sigma y^2)}{(\Delta x)^2} \exp(-v) \frac{\partial^2 u_1}{\partial x^2} - \frac{2\sigma_0\,(1+\sigma-\sigma y^2)}{(\Delta x)^2} \exp(-v)\,(1+y) \frac{dv}{dx} \frac{\partial^2 u_1}{\partial y \partial x}$$

$$+ \frac{4\sigma_0\,(1+\sigma-\sigma y^2)}{h_0^2 \exp(3v)} \frac{\partial^2 u_1}{\partial y^2} - \frac{2\sigma_0\,(1+\sigma-\sigma y-2\sigma y^2)}{(\Delta x)^2} \frac{dv}{dx} \exp(-v) \frac{\partial u_1}{\partial x} - \frac{\sigma_0 8\sigma y}{h_0^2 \exp(3v)} \frac{\partial u_1}{\partial y}$$

$$- \frac{\sigma_0}{(\Delta x)^2} \exp(-v) \left[(1+\sigma-2\sigma-3\sigma y^2) \left(\frac{dv}{dx}\right)^2 + (1+\sigma-\sigma y^2) \frac{d^2 v}{dx^2}\right] u_1 \,. \tag{18}$$

Let us represent the dimensional unknown functions as the sum of the dimensional constant and the dimensionless function:

$$\Delta x = L\,, \quad u_1 = \frac{U_0}{\Delta x} \tilde{u}_1\,, \quad u_2 = \frac{U_0}{\Delta x} \tilde{u}_2\,, \quad p = \rho U_0^2 \tilde{p}\,, \quad G = \frac{g \Delta x}{U_0^2} \tag{19}$$

($\sim$ points to the dimensionless character of the function), previously dividing the two sides of it by $U_0/\Delta x$:

$$\left(\tilde{u}_1 \frac{\partial \tilde{u}_1}{\partial x} + \tilde{u}_2 \frac{\partial \tilde{u}_1}{\partial y} - \tilde{u}_1^2 \frac{\partial v}{\partial x}\right) \exp(-2v) = -\frac{\partial \tilde{p}}{\partial x} + (y+1) \frac{dv}{dx} \frac{\partial \tilde{p}}{\partial x} + G$$

$$+ \frac{\sigma_0\,(1+\sigma-\sigma y^2)}{\Delta x U_0} \exp(-v) \frac{\partial^2 \tilde{u}_1}{\partial x^2} - \frac{2\sigma_0\,(1+\sigma-\sigma y^2)}{\Delta x U_0} \exp(-v)\,(1+y) \frac{dv}{dx} \frac{\partial^2 \tilde{u}_1}{\partial y \partial x}$$

$$+ \frac{4\sigma_0\,(1+\sigma-\sigma y^2)\,\Delta x}{h_0^2 U_0 \exp(3v)} \frac{\partial^2 \tilde{u}_1}{\partial y^2} - \frac{2\sigma_0\,(1+\sigma-\sigma y-2\sigma y^2)}{\Delta x U_0} \frac{dv}{dx} \exp(-v) \frac{\partial \tilde{u}_1}{\partial x} - \frac{\sigma_0 \Delta x 8\sigma y}{h_0^2 U_0 \exp(3v)} \frac{\partial \tilde{u}_1}{\partial y}$$

$$+ \frac{\sigma_0}{\Delta x U_0} \exp(-v) \left[(1+\sigma-2\sigma y-3\sigma y^2) \left(\frac{dv}{dx}\right)^2 + (1+\sigma-\sigma y^2) \frac{d^2 v}{dx^2}\right] \tilde{u}_1 \,. \tag{20}$$

We remove the common factor from all the terms containing derivatives of $\tilde{u}_1$:

$$\left(\tilde{u}_1 \frac{\partial \tilde{u}_1}{\partial x} + \tilde{u}_2 \frac{\partial \tilde{u}_1}{\partial y} - \tilde{u}_1^2 \frac{\partial v}{\partial x}\right) \exp(-2v) = -\frac{\partial \tilde{p}}{\partial x} + (y+1) \frac{dv}{dx} \frac{\partial \tilde{p}}{\partial x} + G$$

$$+ \frac{\sigma_0 \Delta x}{h_0^2 U_0} \left\{ \frac{h_0^2}{(\Delta x)^2} \frac{1+\sigma-\sigma y^2}{U_0} \exp(-v) \frac{\partial^2 \tilde{u}_1}{\partial x^2} - \frac{h_0^2}{(\Delta x)^2} 2\,(1+\sigma-\sigma y^2) \exp(-v)\,(1+y) \frac{dv}{dx} \frac{\partial^2 \tilde{u}_1}{\partial y \partial x} \right.$$

$$+\frac{4\,(1+\sigma-\sigma y^{2})}{\exp\,(3v)}\frac{\partial^{2}\tilde{u}_1}{\partial y^{2}}-\frac{h_0^{2}}{(\Delta x)^{2}}\,2\,(1+\sigma-\sigma y-2\sigma y^{2})\frac{dv}{dx}\exp\,(-\,v)\frac{\partial\tilde{u}_1}{\partial x}-\frac{8\sigma y}{\exp\,(3v)}\frac{\partial\tilde{u}_1}{\partial y}$$

$$+\frac{h_0^{2}}{(\Delta x)^{2}}\exp\,(-\,v)\left[(1+\sigma-2\sigma y-3\sigma y^{2})\left(\frac{dv}{dx}\right)^{2}+(1+\sigma-\sigma y^{2})\frac{d^{2}v}{dx^{2}}\right]\tilde{u}_1\Bigg\}\,.$$

Then, in accordance with (17), we have

$$\tilde{u}_1\frac{\partial\tilde{u}_1}{\partial x}+\tilde{u}_2\frac{\partial\tilde{u}_1}{\partial y}-\tilde{u}_1^{2}\frac{dv}{dx}=-\exp\,(-\,2v)\frac{\partial\tilde{p}}{\partial x}+(y+1)\exp\,(2v)\frac{dv}{dx}\frac{\partial\tilde{p}}{\partial x}+G\exp\,(2v)$$

$$+\,4\left(\frac{\sigma_0}{h_0U_0}\right)\left(\frac{\Delta x}{h_0}\right)\exp\,(-\,v)\left\{(1+\sigma-\sigma y^{2})\frac{\partial^{2}\tilde{u}_1}{\partial y^{2}}-2\sigma y\frac{\partial\tilde{u}_1}{\partial y}\right\}. \tag{21}$$

By analogy with (16), we obtain

$$(1+y)\frac{dv}{dx}\left(\tilde{u}_1\frac{\partial\tilde{u}_1}{\partial x}+\tilde{u}_2\frac{\partial\tilde{u}_1}{\partial y}\right)+\tilde{u}_1\frac{\partial\tilde{u}_2}{\partial x}+\tilde{u}_2\frac{\partial\tilde{u}_2}{\partial y}+(1+y)\frac{d^{2}v}{dx^{2}}\tilde{u}_1^{2}+\tilde{u}_1\tilde{u}_2\frac{dv}{dx}=-\,\frac{4\,(\Delta x)^{2}}{h_0^{2}}\frac{\partial\tilde{p}}{\partial y}$$

$$+\,4\left(\frac{\sigma_0}{h_0U_0}\right)\frac{\Delta x}{h_0}\Bigg\{\exp\,(-\,v)\,(1+\sigma-\sigma y^{2})\,(1+y)\frac{dv}{dx}\frac{\partial^{2}\tilde{u}_1}{\partial y^{2}}+\exp\,(-\,v)\,(1+\sigma-\sigma y^{2})\frac{\partial^{2}\tilde{u}_2}{\partial y^{2}}$$

$$+\,4\exp\,(v)\,(1+\sigma-\sigma y-2\sigma y^{2})\frac{dv}{dx}\frac{\partial\tilde{u}_1}{\partial y}-2\sigma y\exp\,(v)\frac{\partial\tilde{u}_2}{\partial y}+2y\sigma\exp\,(-\,v)\frac{dv}{dx}\tilde{u}_1\Bigg\}. \tag{22}$$

Using condition (17), just as in the classical case (dividing both sides by $(\Delta x)^2/h_0^2$), we can reduce Eq. (22) to the equation

$$\frac{\partial\tilde{p}}{\partial y}(x,y)=0\,,\quad 0\le x\le\frac{L}{\Delta x}=l\,,\quad -1<y<1\,, \tag{23}$$

thus considering that $\tilde{p}$ is dependent only on the variable x. The available feature is noteworthy. Generally speaking, the asymptotic approximation (23) of Eq. (22) holds only within $-1 < y < 1$. If, as a boundary condition, we take (as is assumed)

$$\frac{\partial p}{\partial y}(\breve{x},h\,(\breve{x}))=0\,,\quad 0\le\breve{x}\le L\,,$$

whence, on the basis of (10), we have

$$\frac{\partial\tilde{p}}{\partial y}(x,1)=0\,,\quad 0\le x\le l\,, \tag{24}$$

then, at the boundary $y = 1$, we should consider

$$2\frac{dv}{dx}\left(\tilde{u}_1\frac{\partial\tilde{u}_1}{\partial x}+\tilde{u}_2\frac{\partial\tilde{u}_1}{\partial y}\right)+\tilde{u}_1\frac{\partial\tilde{u}_2}{\partial x}+\tilde{u}_2\frac{\partial\tilde{u}_2}{\partial y}+2\frac{d^{2}v}{dx^{2}}\tilde{u}_1^{2}+\tilde{u}_1\tilde{u}_2\frac{dv}{dx}$$

$$= 4\left(\frac{\sigma_0}{h_0 U_0}\right)\frac{\Delta x}{h_0}\left\{\exp(-v)\,2\,\frac{dv}{dx}\frac{\partial^2 \tilde{u}_1}{\partial y^2} + \exp(-v)\,\frac{\partial^2 \tilde{u}_2}{\partial y^2} + 4\,(1-2\sigma)\exp(v)\,\frac{dv}{dx}\frac{\partial \tilde{u}_1}{\partial y}\right.$$

$$\left. - 2\sigma\exp(v)\,\frac{\partial \tilde{u}_2}{\partial y} + 2\sigma\exp(-v)\,\frac{dv}{dx}\,\tilde{u}_1\right\} \qquad (25)$$

instead of (23). Since this equation is considered on the vanishing region of the boundary $y = 1$ which is a streamline, we may disregard the terms containing $\partial^2\tilde{u}_1/\partial y^2$ and $\partial^2\tilde{u}_2/\partial y^2$ in it.

Noting that the relation between the numbers

$$\mathrm{Re}_0 = \frac{h_0 U_0}{\sigma_0} \quad \text{and} \quad \frac{\Delta x}{h_0} \qquad (26)$$

is quite substantial in investigating system (14), (21), and (25), we introduce the constant

$$\chi = \log_{\mathrm{Re}_0}\left(\frac{\Delta x}{h_0}\right). \qquad (27)$$

Then the dimensionless system under study can be written in the form

$$\frac{\partial \tilde{u}_1}{\partial x} + \frac{\partial \tilde{u}_2}{\partial y} = 0\,, \qquad (28)$$

$$\tilde{u}_1\frac{\partial \tilde{u}_1}{\partial x} + \tilde{u}_2\frac{\partial \tilde{u}_1}{\partial y} - \tilde{u}_1^2\frac{dv}{dx} = -\exp(2v)\,\frac{d\tilde{p}}{dx} + G\exp(2v)$$

$$+ 4\mathrm{Re}_0^{\chi-1}\exp(-v)\left\{(1+\sigma-\sigma y^2)\,\frac{\partial^2\tilde{u}_1}{\partial y^2} - 2\sigma y\,\frac{\partial \tilde{u}_1}{\partial y}\right\}, \quad 0 \le x \le l\,, \quad -1 \le y \le 1\,; \qquad (29)$$

$$2\mathrm{Re}_0^{1-\chi}\frac{dv}{dx}\left(\tilde{u}_1\frac{\partial \tilde{u}_1}{\partial x} + \tilde{u}_2\frac{\partial \tilde{u}_1}{\partial y}\right) + \mathrm{Re}_0^{1-\chi}\,\tilde{u}_1\frac{\partial \tilde{u}_2}{\partial x} + \mathrm{Re}_0^{1-\chi}\,\tilde{u}_2\frac{\partial \tilde{u}_2}{\partial y}$$

$$+ 2\mathrm{Re}_0^{1-\chi}\frac{d^2 v}{dx^2}\,\tilde{u}_1^2 + \mathrm{Re}_0^{1-\chi}\,\tilde{u}_1\tilde{u}_2\frac{dv}{dx} = 16\,(1-2\sigma)\exp(v)\,\frac{dv}{dx}\frac{\partial \tilde{u}_1}{\partial y} + 8\sigma\exp(v)\,\frac{\partial \tilde{u}_1}{\partial x}$$

$$+ 8\sigma\exp(-v)\,\frac{dv}{dx}\,\tilde{u}_1\,, \quad 0 \le x \le l\,, \quad y = 1\,. \qquad (30)$$

Let us pass on to the method of solution of this system with the adhesion condition at the boundary with a solid wall:

$$u_1 = 0\,, \quad u_2 = 0\,, \quad 0 \le x \le l\,, \quad y = 0\,. \qquad (31)$$

For this purpose we show that passage to the new variables and unknowns (10)–(12) enables us to preserve the entire formal part of the method of equal-flow-rate surfaces [1]. It is based on the assumption that, in a plane stationary film flow described in coordinates (x, y), we can single out the series of streamlines $\{\breve{y} = \breve{y}_k(\breve{x})\}_{k=0}^{N}$, i.e., the lines on which we have the equality

$$U_2\,(\breve{x}, \breve{y}_k\,(\breve{x})) = \frac{d\breve{y}_k\,(\breve{x})}{d\breve{x}}\,U_1\,(\breve{x}, \breve{y}_k\,(\breve{x}))\,, \tag{32}$$

dividing the entire flow into the subflows (between two neighboring lines of the series) in which the flow rate of the liquid per unit time remains the same (i.e., independent of $\breve{x}$) for any cross section $\breve{x} \equiv$ const:

$$\int\limits_{\breve{y}_k(\breve{x})}^{\breve{y}_{k+1}(\breve{x})} U_1\,(\breve{x}, s)\,ds \equiv \text{const} \Leftrightarrow \frac{d}{d\breve{x}} \int\limits_{\breve{y}_k(\breve{x})}^{\breve{y}_{k+1}(\breve{x})} U_1\,(\breve{x}, s)\,ds = 0\,. \tag{33}$$

Curves into which the series $\{\breve{y} = \breve{y}_k(\breve{x})\}_{k=0}^{N}$ goes over on substitution of variables (10) have the form

$$\left\{ y_k = \frac{2}{h_0}\,\breve{y}_k\,(x\Delta x)\,\exp\,(-\,v\,(x)) - 1 \right\}_{k=0}^{N}\,.$$

For this series, in accordance with (11), equality (32) will become the relation

$$\frac{1 + y_k}{2}\,\exp\,(v)\,\frac{dv}{dx}\,w_1 + \frac{\exp\,(v)}{2}\,w_2 = \frac{d}{dx}\left(\frac{(1 + y_k)}{2}\,\exp\,(v)\right) w_1 \Leftrightarrow w_2\,\frac{dy_k}{dx}\,w_1\,,$$

which, according to (12), is equivalent to the equality

$$\tilde{u}_2 = \frac{dy_k}{dx}\,\tilde{u}_1\,. \tag{34}$$

Expression (33) entirely retains its formal form on passage to the new variables and unknowns (10)–(12). Indeed, since

$$\int\limits_{\breve{y}_k(\breve{x})}^{\breve{y}_{k+1}(\breve{x})} U_1\,(\breve{x}, \breve{y})\,d\breve{y} = \int\limits_{y_k(x)}^{y_{k+1}(x)} \Delta x\,\exp\,(-\,v\,(x))\,u_1\,(x, y)\,\frac{h_0}{2}\,\exp\,(v\,(x))\,dy = \frac{U_0 h_0}{2} \int\limits_{y_k(x)}^{y_{k+1}(x)} \tilde{u}_1\,(x, y)\,dy = \text{const}\,,$$

we have

$$\frac{d}{dx} \int\limits_{y_k(x)}^{y_{k+1}(x)} \tilde{u}_1\,(x, y)\,dy = 0\,. \tag{35}$$

Following the method of equal-flow-rate surfaces, we compose a system of $2(N - 1)$ equations, preintroducing the notation $u_{1,k}(x) = u_1(x, y_k(x))$:

$$\begin{gathered} 4\,(\sigma\,(1 - y^2) + 1)\,\frac{\partial^2 \tilde{u}_1}{\partial y_k^2}\,(x, y_k) - 8\sigma y\,\frac{\partial \tilde{u}_1}{\partial y_k}\,(x, y_k) + \mathrm{Re}_0^{1-\chi}\,\exp\,(v)\,\tilde{u}_{1,k}^2\,\frac{dv}{dx} \\ -\,\mathrm{Re}_0^{1-\chi}\,\exp\,(3v)\,\frac{d\tilde{p}}{dx} + \mathrm{Re}_0^{1-\chi}\,G\,\exp\,(3v) = \mathrm{Re}_0^{1-\chi}\,\exp\,(v)\,\tilde{u}_{1,k}\,\frac{d\tilde{u}_{1,k}}{dx}\,; \end{gathered} \tag{36}$$

$$\frac{dy_k(x)}{dx} = \frac{dy_{k-1}(x)}{dx} - \frac{\dfrac{d\tilde{u}_{1,k}(x)}{dx} + \dfrac{d\tilde{u}_{1,k-1}(x)}{dx}}{\tilde{u}_{1,k}(x) + \tilde{u}_{1,k-1}(x)} \left(y_k(x) - y_{k-1}(x)\right), \quad k = 1, 2, ..., N-1 .$$

This system is open, since contains $2N$ unknowns. It is closed by addition of equations determined in a certain small vicinity of the straight line $y = 1$. Continuing the first group of equations (36) and disregarding (just as in deriving (25)) the term with $\partial^2\tilde{u}_1/\partial y^2$, we obtain

$$-8\sigma\frac{\partial\tilde{u}_1}{\partial y_k}(x, 1) + \mathrm{Re}_0^{1-\chi}\exp(v)\,\tilde{u}_{1,N}^2\frac{dv}{dx} - \mathrm{Re}_0^{1-\chi}\exp(3v)\frac{d\tilde{p}}{dx} + \mathrm{Re}_0^{1-\chi}G\exp(3v)$$

$$= \mathrm{Re}_0^{1-\chi}\exp(v)\,\tilde{u}_{1,N}\frac{d\tilde{u}_{1,N}}{dx} . \tag{37}$$

Equation (37) contains one more unknown $\tilde{u}_{1,N}$. Continuing the second group of equations and taking into account that $y_N = 1$ and $dy_N/dx = 0$, we have

$$\frac{\dfrac{dy_{N-1}(x)}{dx}}{1 - y_{N-1}(x)} = \frac{\dfrac{d\tilde{u}_{1,N}(x)}{dx} + \dfrac{d\tilde{u}_{1,N-1}(x)}{dx}}{\tilde{u}_{1,N}(x) + \tilde{u}_{1,N-1}(x)} . \tag{38}$$

This equation is easily solved for $\tilde{u}_{1,N}$

$$\tilde{u}_{1,N}(x) = \left(\frac{1 - y_{N-1}(0)}{1 - y_{N-1}(x)}\right)\left(\tilde{u}_{1,N}(0) + \tilde{u}_{1,N-1}(0)\right) - \tilde{u}_{1,N-1}(x) . \tag{39}$$

Finally, taking into account that

$$\frac{\partial u_1}{\partial y_N}(x, y_N) = \frac{du_{1,N}}{dx}(x) , \quad \tilde{u}_2(x, 1) = \frac{\partial\tilde{u}_2}{\partial x}(x, 1) = 0 , \quad 0 \le x \le l ,$$

we can write Eq. (30) in the form

$$8(1 - 2\sigma)\exp(v)\frac{dv}{dx}\frac{\partial\tilde{u}_1}{\partial y}(x, 1) - \mathrm{Re}_0^{1-\chi}\frac{d^2v}{dx^2}\tilde{u}_1^2 + 4\sigma\exp(-v)\frac{dv}{dx}\tilde{u}_1$$

$$= \left(\mathrm{Re}_0^{1-\chi}\tilde{u}_1 - 4\sigma\exp(-v)\right)\frac{dv}{dx}\frac{d\tilde{u}_1}{dx} . \tag{40}$$

The three equations (37), (38) (or (39)), and (40) containing only one complementary unknown complete system (36) to a closed system.

In closing this section, we note that the values Δx = 2 m, $h_0 \approx 0.00086$ m, and $\chi \approx 1.3228$ have been taken in the above calculations.

Thermophysical Part of the Model. We have indicated above a substitution of variables in Eqs. (1)–(4) such that the domain of variation in spatial variables becomes a rectangle. However, for the model's part in question, it is better to take the equivalent modification of this substitution with a rectangular domain of variation in spatial variables, too,

$$x = \breve{x} , \quad y = \frac{\breve{y}}{h(\breve{x})} ,$$

in accordance with which we have

$$W_1 = w_1 \,, \quad W_2 = y \frac{dh}{d\tilde{x}} w_1 + h w_2 \,.$$

The relationship between w_i and the $\tilde{u}_i$ values computed above is trivial. Furthermore, with the aim of allowing for the turbulent character of film motion in this part of the problem, too, we consider the case where

$$D_\mathrm{a} = D_\mathrm{b} = D\,(1 + \mathrm{TD}\,(y - y^2)) \,, \quad a_\mathrm{c} = a_{\mathrm{c}0}\,(1 + \mathrm{TL}_\mathrm{c}\,(y - y^2)) \,, \quad a_\mathrm{w} = a_{\mathrm{w}0}\,(1 + \mathrm{TL}_\mathrm{w}\,(-y - y^2)) \,,$$

where D, $a_{\mathrm{c}0}$, and $a_{\mathrm{w}0}$ are respectively the molecular diffusion and thermal diffusivities, and the constants TD and TL are determined, in accordance with [1], as

$$\mathrm{TB} = 0.0014 \frac{\rho}{\nu} \mathrm{Re}^{77/30} g^{1/3} (\sigma^\mathrm{kin})^{4/3} \,, \quad \mathrm{TD} = \mathrm{TB} \frac{\sigma^\mathrm{kin}}{D} \,, \quad \mathrm{TL} = \mathrm{TB} \frac{\sigma^\mathrm{kin}}{a} \,.$$

In this part of the model, intermediate transformations are more simple than those in the previous part. Therefore, we can drop them, passing over immediately to a dimensionless form. For this purpose we set

$$T_\mathrm{R} = T_0 + \frac{Q_\mathrm{c} C_{\mathrm{a}0}}{c_\mathrm{c} \rho_\mathrm{c}} \,, \quad \theta = \frac{T - T_0}{T_0} \,, \quad \theta_0 = \frac{T_0 - T_\mathrm{R}}{T_\mathrm{R}} \,, \quad \Delta_\mathrm{a} = \frac{R T_\mathrm{R}}{E_\mathrm{a}} \,, \quad \Delta_\mathrm{b} = \frac{R T_\mathrm{R}}{E_\mathrm{b}} \,,$$

$$\eta = \frac{C_\mathrm{a}}{C_{\mathrm{a}0}} \,, \quad \varphi = \frac{C_\mathrm{b}}{C_{\mathrm{a}0}} \,, \quad a_\mathrm{c} = \frac{\lambda_\mathrm{c}}{c_\mathrm{c} \rho_\mathrm{c}} \,, \quad a_\mathrm{w} = \frac{\lambda_\mathrm{w}}{c_\mathrm{w} \rho_\mathrm{w}} \,, \quad \Delta t = \frac{1}{K_\mathrm{a} C_{\mathrm{a}0}} \exp\left(\frac{1}{\Delta_\mathrm{a}}\right), \tag{41}$$

$$\Delta x = \sqrt{D_\mathrm{a} \Delta t} \,, \quad \Delta u = \frac{\Delta x}{\Delta t} \,, \quad \tau = \frac{t}{\Delta t} \,, \quad \xi = \frac{x}{\Delta x} \,, \quad l = \frac{L}{\Delta x} \,, \quad f_\mathrm{c} = \frac{\Delta x}{h_{\mathrm{c}0}} \,,$$

$$f_\mathrm{w} = \frac{\Delta x}{h_{\mathrm{w}0}} \,, \quad z_\mathrm{a} = \frac{T_\mathrm{R} - T_{\mathrm{c}0}}{T_\mathrm{R}} \,, \quad z_\mathrm{b} = K_\mathrm{b} \exp\left(-\frac{1}{\Delta_\mathrm{b}}\right) \Delta t \,.$$

The model's thermochemical part made dimensionless has the form

$$\frac{\partial \eta}{\partial \tau} = H^0 \frac{\partial^2 \eta}{\partial \xi^2} + H^1 \frac{\partial^2 \eta}{\partial y \partial \xi} + H^2 \frac{\partial^2 \eta}{\partial y^2} + H^3 \frac{\partial \eta}{\partial \xi} + H^4 \frac{\partial \eta}{\partial y} - \eta \varphi \exp\left(\frac{\theta}{\Delta_\mathrm{a}(\theta + 1)}\right),$$

$$\frac{\partial \varphi}{\partial \tau} = H^0 \frac{\partial^2 \varphi}{\partial \xi^2} + H^1 \frac{\partial^2 \varphi}{\partial y \partial \xi} + H^2 \frac{\partial^2 \varphi}{\partial y^2} + H^3 \frac{\partial \varphi}{\partial \xi} + H^4 \frac{\partial \varphi}{\partial y} - z_\mathrm{b} \varphi \exp\left(\frac{\theta}{\Delta_\mathrm{b}(\theta + 1)}\right), \quad 0 \le x \le l \,, \quad 0 \le y \le 1 \,; \tag{42}$$

$$\frac{\partial \theta}{\partial \tau} = H_T^0 \frac{\partial^2 \theta}{\partial \xi^2} + H_T^1 \frac{\partial^2 \theta}{\partial y \partial \xi} + H_T^2 \frac{\partial^2 \theta}{\partial y^2} + H_T^3 \frac{\partial \theta}{\partial \xi} + H_T^4 \frac{\partial \theta}{\partial y} + z_\mathrm{a} \eta \varphi \exp\left(\frac{\theta}{\Delta_\mathrm{a}(\theta + 1)}\right), \quad 0 \le x \le l \,, \quad -1 \le y \le 1 \,.$$

The smooth coefficients H^i (i = 0, 1, 2, 3, and 4) and piesewise-smooth (discontinuity of the first kind on the barrier separating water and the reacting mixture) coefficients H_T^i (i = 0, 1, 2, 3, and 4) appearing in (42) are determined from the formulas

$$r_0 = \frac{D}{D_*} \,, \quad r_1 = \frac{D}{D_*} \mathrm{TD} \,, \quad r_{\mathrm{w}0} = \frac{a_{\mathrm{w}0}}{a_*} \,, \quad r_{\mathrm{w}1} = \frac{a_{\mathrm{w}0}}{a_*} \mathrm{TL}_\mathrm{w} \,, \quad r_{\mathrm{c}1} = \frac{a_{\mathrm{c}0}}{a_*} \,, \quad r_{\mathrm{c}1} = \frac{a_{\mathrm{c}0}}{a_*} \mathrm{TL}_\mathrm{c} \,;$$

$$H^0 = r_0 + r_1\,(y - y^2)\,;\quad H^1 = -\,2y\,\frac{dv_\mathrm{c}}{d\xi}\,H^0\,;\quad H^2 = \left(y^2\left(\frac{dv_\mathrm{c}}{d\xi}\right)^2 + f_\mathrm{c}^2\exp\,(-\,2v_\mathrm{c})\right)H^0\,;$$

$$H^3 = -\,r_1\,(1 - 2y)\,y\,\frac{dv_\mathrm{c}}{d\xi} - u_1\,;$$

$$H^4 = yH^0\left(\left(\frac{dv_\mathrm{c}}{d\xi}\right)^2 - \frac{d^2v_\mathrm{c}}{d\xi^2}\right) + r_1\,(1 - 2y)\left(y^2\left(\frac{dv_\mathrm{c}}{d\xi}\right)^2 + f_\mathrm{c}^2\exp\,(-\,2v_\mathrm{c})\right);$$

$$H_T^0 = \begin{cases} r_{\mathrm{w}0} - r_{\mathrm{w}1}\,(y - y^2)\,, & -\,1 \le y < 0\,, \\ r_{\mathrm{c}0} + r_{\mathrm{c}1}\,(y - y^2)\,, & 0 < y \le 1\,; \end{cases} \qquad H_T^1 = \begin{cases} -\,2y\,\dfrac{dv_\mathrm{w}}{d\xi}\left(r_{\mathrm{w}0} - r_{\mathrm{w}1}\,(y - y^2)\right), & -\,1 \le y < 0\,, \\ -\,2y\,\dfrac{dv_\mathrm{c}}{d\xi}\left(r_{\mathrm{c}0} + r_{\mathrm{c}1}\,(y - y^2)\right), & 0 < y \le 1\,; \end{cases} \tag{43}$$

$$H_T^2 = \begin{cases} \left(y^2\left(\dfrac{dv_\mathrm{w}}{d\xi}\right)^2 + f_\mathrm{w}^2\exp\,(-\,2v_\mathrm{w})\right)\left(r_{\mathrm{w}0} - r_{\mathrm{w}1}\,(y - y^2)\right), & -\,1 \le y < 0\,; \\ \left(y^2\left(\dfrac{dv_\mathrm{c}}{d\xi}\right)^2 + f_\mathrm{c}^2\exp\,(-\,2v_\mathrm{c})\right)\left(r_{\mathrm{c}0} + r_{\mathrm{c}1}\,(y - y^2)\right), & 0 < y \le 1\,; \end{cases}$$

$$H_T^3 = \begin{cases} r_{\mathrm{w}1}\,(1 + 2y)\,y\,\dfrac{dv_\mathrm{w}}{d\xi} - u_{1\mathrm{w}}\,, & -\,1 \le y < 0\,; \\ -\,r_{\mathrm{c}1}\,(1 - 2y)\,y\,\dfrac{dv_\mathrm{c}}{d\xi} - u_{1\mathrm{c}}\,, & 0 < y \le 1\,; \end{cases}$$

$$H_T^4 = \begin{cases} y\left(r_{\mathrm{w}0} - r_{\mathrm{w}1}\,(y - y^2)\right)\left(\left(\dfrac{dv_\mathrm{w}}{d\xi}\right)^2 - \dfrac{d^2v_\mathrm{w}}{d\xi^2}\right) - r_{\mathrm{w}1}\,(1 + 2y)\left(y^2\left(\dfrac{dv_\mathrm{w}}{d\xi}\right)^2 + f_\mathrm{w}^2\exp\,(-\,2v_\mathrm{w})\right), & -\,1 \le y < 0\,; \\ y\left(r_{\mathrm{c}0} + r_{\mathrm{c}1}\,(y - y^2)\right)\left(\left(\dfrac{dv_\mathrm{c}}{d\xi}\right)^2 - \dfrac{d^2v_\mathrm{c}}{d\xi^2}\right) + r_{\mathrm{c}1}\,(1 - 2y)\left(y^2\left(\dfrac{dv_\mathrm{c}}{d\xi}\right)^2 + f_\mathrm{c}^2\exp\,(-\,2v_\mathrm{c})\right), & 0 < y \le 1\,. \end{cases}$$

Numerical Investigation of the Model. Numerical calculation was carried out for the following values of the constants: $C_{\mathrm{a}0} = 1000$ mole/m^3, $C_{\mathrm{b}0} = 10$ mole/m^3, $\rho_\mathrm{a} = 635$ kg/m^3, $\rho_\mathrm{b} = 1000$ kg/m^3, $c_\mathrm{c} = 2174$ J/(kg·K), $c_\mathrm{w} = 4187$ J/(kg·K), $T_0 = 293$ K, $R = 8.3144$ J/(mole·K), $E_\mathrm{a} = 12{,}560$ J/mole, $E_\mathrm{b} = 16{,}747$ J/mole, $K_\mathrm{a} = 2.95 \cdot 10^4$ m^3/(mole·sec), $K_\mathrm{b} = 3.37 \cdot 10^5$ m^3/(mole·sec), $Q_\mathrm{c} = 5.400 \cdot 10^4$ J/mole, and $a_\mathrm{w} = a_\mathrm{c} = a_* = 0.025$ m^2/sec.

First we calculated the motion of the films independently from the thermochemical problem. The calculation results coincided with those obtained by another method [1]. The advantage of the procedure discussed is that it is suitable for investigation of the hydrodynamics of a film-type reactor simultaneously with the thermochemical problem.

The thermochemical part of the model was investigated using the variable-direction method [4]. The sources and the finite-difference analog of a mixed derivative were universally present for any time half-step on the right-hand side. The leading part on the left-hand side was played by the finite-difference analogs of the operators $H^0\dfrac{\partial^2}{\partial\xi^2} + H^3\dfrac{\partial}{\partial\xi}$ and $H^2\dfrac{\partial^2}{\partial y^2} + H^4\dfrac{\partial}{\partial y}$ respectively denoted by Λ_ξ and Λ_y and alternately replacing one another. The action of the first operator on the grid function $\psi_{i,j}$, where the segment [0, 1] or [−1, 1] (variable y) is uniformly broken with a step Δy in i, and $[0, l]$ (variable ξ) is broken with a step $\Delta\xi$ in j, has the form

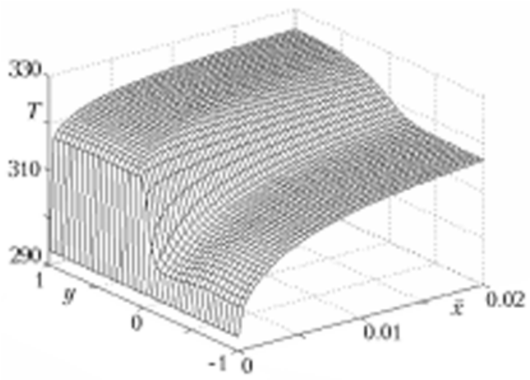

Fig. 1. Temperature distribution in the reacting-mixture film–water film system. T, K; $\breve{x}$, m.

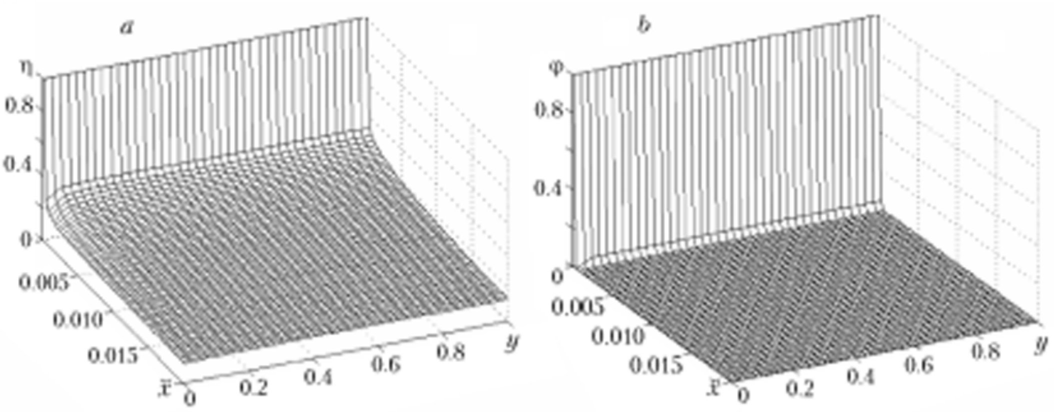

Fig. 2. Distribution of the dimensionless concentration of the monomer (a) and the catalyst (b) in the film of a reacting mixture. $\breve{x}$, m.

$$\left(\frac{H^{3}_{i,j+1}}{2\Delta\xi}+\frac{H^{0}_{i,j}}{(\Delta\xi)^{2}}\right)\psi_{i,j+1}-\left(\frac{2H^{0}_{i,j}}{(\Delta\xi)^{2}}\right)\psi_{i,j}+\left(\frac{2H^{0}_{i,j}}{(\Delta\xi)^{2}}-\frac{H_{i,j-1}}{2\Delta\xi^{3}}\right)\psi_{i,j-1}.$$

The action of the operator Λ_y is written as

$$\left(\frac{H^{4}_{i+1,j}}{2\Delta y}\right)\psi_{i,j+1}-\left(\frac{2H^{2}_{i,j}}{(\Delta y)^{2}}\right)\psi_{i,j}+\left(\frac{H^{2}_{i,j}}{(\Delta y)^{2}}-\frac{H_{i-1,j}}{2\Delta y}\right)\psi_{i-1,j}.$$

As the calculations have shown, the relations between the preexponents K_a and K_b are basic in this part of the problem. The situation where K_a is an order of magnitude smaller than K_b is presented in Fig. 1. With the selected values of the parameters, the temperature in the reaction zone grows by ~50°C (Fig. 1). As follows from the same plot of temperature in both films, the water film moving faster (because of its heavier weight) removes a substantial part of heat from the reacting film. The plots of concentrations of the starting reagents (Fig. 2a) and the catalyst (active sites [4]) (Fig. 2b) demonstrate that the model description selected and the parametric region place the active-reaction zone in the beginning of the system; the system itself has a small width. As is demonstrated by calculations for the considered parameters of the problem, the small thickness of the reacting film and the excess of the rate of chemical decrease in the catalyst over the velocity of film flow represent the necessary conditions under which the reaction will occur mainly in the small vicinity of the reactor inlet. The relation of the rate of chemical decrease in the catalyst and the velocity of film flow calls for additional experimental investigations.

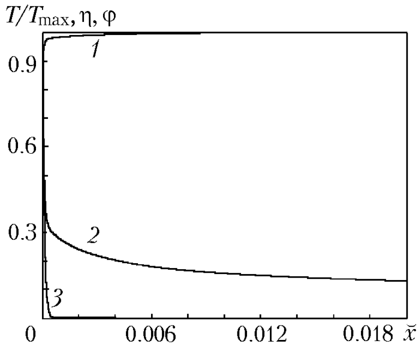

Fig. 3. Averaged (over y) distributions normalized to their maxima of the: 1) temperature; 2) concentration of the monomer, and 3) concentration of the catalyst. $\breve{x}$, m.

Figure 3 shows, in combination, the distributions of the concentrations of the starting components and the catalyst and of the temperature, averaged over y and normalized to their maximum values. It is precisely this figure that enables us to gain a complete impression of the process. In particular, it follows from the figure that in the case where the mixture begins to actively react at room temperature most of the reaction will occur at lower temperatures than those at the system's outlet. This fact for such mixtures essentially follows from the structural features of film-type flow reactors with cooling. Despite the fact that fast exothermic reactions enjoy wide application in chemical engineering, their kinetics has yet to be adequately studied.

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NOTATION

$a = \lambda/(c\rho)$, thermal diffusivity of the mixture, m^2/sec; c, specific heat of the mixture, J/(kg·K); C, dimensional concentration of the substance, mole/m^3; D, diffusion coefficient, m^2/sec; E, activation energy of the reaction, J/mole; f, dimensionless parameter; g, free-fall acceleration, 9.8 m/sec^2; $G = g\Delta x/U_0^2$, dimensionless constant; h, thickness of the flowing-down film, m; H, dimensionless coefficient of system (42); K, kinetic reaction-rate constant (for the monomer, $\text{m}^3/(\text{mole·sec})$; for the catalyst, 1/sec); L, size of the entire system along the Ox axis (≡ length of the entire system), m; $l = L/(\Delta x)$, dimensionless length of the entire system; p, pressure, N/m^2; $\tilde{p}$, dimensionless pressure; Q, thermal effect of the reaction, J/mole; R, universal gas constant, J/(mole·K); $\text{Re}_0 = h_0U_0/\sigma_0$, dimensionless constant; s, integration variable; S, flow rate in the flowing-film cross section, m^2/sec; $\breve{t}$, time coordinate, sec; t, dimensionless time coordinate; T, temperature, K; T_{R}, characteristic reaction temperature, K (see (41)); $\text{TB} = 0.0014\frac{\rho}{\nu}\text{Re}^{77/30}g^{1/3}(\sigma^{\text{kin}})^{4/3}$, $\text{TD} = \text{TB}\,\frac{\sigma^{\text{kin}}}{D}$, and $\text{TL} = \text{TB}\,\frac{\sigma^{\text{kin}}}{a}$, constants; $v = v(x) = \ln\left(\frac{h(x)}{h_0}\right)$, logarithm of the thickness of the flowing-down film normalized to its (initial) thickness at entry into the system h_0; $\mathbf{U} = (U_1, U_2)$, film velocity in a unified representation of the hydrodynamic part of the problem, m/sec; $\mathbf{u} = (u_1, u_2)$, film velocity in a unified representation of the hydrodynamic part of the problem on passage to new variables and unknowns, 1/sec; $(\tilde{u}_1, \tilde{u}_2)$, dimensionless film velocity in a unified representation of the hydrodynamic part of the problem on passage to new variables and unknowns; $u_{1,k}(x) = u_1(x, y_k(x))$, series of unknown functions in problem (36); U_0, film velocity at entry into the system, m/sec; $\mathbf{V} = (V_1, V_2)$, velocity of flowdown of the water film, m/sec; $\mathbf{W} = (W_1, W_2)$, velocity of flowdown of the reacting-mixture film, m/sec; $\mathbf{w} = (w_1, w_2)$, film velocity in a unified representation of the hydrodynamic part of the problem on passage to new spatial variables, 1/sec; $(\breve{x}, \breve{y})$, space coordinates, m; (x, y), dimensionless space coordinates; $\left\{ y_k = \frac{2}{h_0} \breve{y}_k(x \cdot \Delta x) \exp(-v(x)) - 1 \right\}_{k=0}^{N}$, series of streamlines of a unified system on passage to new variables and unknowns; $\{\breve{y} = \breve{y}_k(\breve{x})\}_{k=0}^{N}$, series of streamlines of the unified system (8); z, dimensionless preexponent (see (41)); $\Delta_{\mathrm{a}} = RT_{\mathrm{R}}/E_{\mathrm{a}}$ and $\Delta_{\mathrm{b}} = RT_{\mathrm{R}}/E_{\mathrm{b}}$, dimensionless parameters; $\Delta t = \frac{1}{K_{\mathrm{a}} C_{\mathrm{a}0}} \exp\left(\frac{1}{\Delta_{\mathrm{a}}}\right)$, characteristic reaction time of the volume element, sec; Δx, scale of the hydrodynamic problem of $\tilde{x}$ or spatial scale of the thermal problem, equal to $\sqrt{D_{\mathrm{a}} \Delta t}$, m; η, dimensionless concentration of the reagents; θ, dimensionless temperature; λ, thermal conductivity of the mixture, J/(m·sec·K); ν, surface tension, N/m; ξ, dimensionless space coordinate in the thermal part of the problem; ψ_{ij}, arbitrary grid function; ρ, density, kg/m^3; σ, viscosity, kg/(m·sec) or the dimensionless constant σ_1/σ_0 (see (9)); τ, dimensionless time coordinate; φ, dimensionless concentration of the catalyst; $\chi = \log_{\mathrm{Re}_0}\left(\frac{\Delta x}{h_0}\right)$, dimensionless parameter. Superscripts: kin and turb, molecular and turbulent components; 0, 1, 2, 3, and 4, number of the dimensionless coefficient in system (42). Subscripts; a, system of parameters of the starting reagents; b, system of parameters of the catalyst; c, system of parameters of the total mixture; i, number of the computational-grid node along the Oy axis; j, number of the computational-grid mode along the Oξ axis; k, number of the streamline to which the parameter belongs; R, temperature constant (see (41)); T, belonging to the dimensionless coefficients of the heat-conduction equation of system (42); w, water; 0, value of the characteristic at entry into the reactor (i.e., at the point $\tilde{x} = 0$) (see (9) for σ, (26) for Re, and (43) for r)); 1 and 2, belonging to the space coordinates along x or along y respectively (see (9) for σ and (43) for r); *, selected constant of rendering quantities dimensionless.

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