TRANSFER PROCESSES IN RHEOLOGICAL MEDIA

INFLUENCE OF VARIOUS FACTORS ON THE FLOW OF A CHEMICALLY REACTIVE NON-NEWTONIAN FLUID IN A PLANE CHANNEL

A. V. Baranov

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A study has been made of the flow of a non-Newtonian polymer medium in a plane channel and of heat transfer in it with boundary conditions of the first kind for small Reynolds numbers and a large Péclet number with the Ellis rheological model with a viscosity dependent on the temperature, pressure, and degree of chemical conversion of the medium. Consideration was given to the flow of a high-viscosity medium with chemical reactions leading to an abrupt increase in its viscosity for whose mathematical description the authors used a model that included the kinetic chemical-reaction equation and the energy equation with a dissipative term. Significant influence of various factors on the formation and rate of growth of the solidified wall layer in such flow has been shown. The problem has been solved numerically by the finite-difference method according to the iterative scheme.

Introduction. The present work is sequel to [1] where numerous investigations into the processes of flow of non-Newtonian media in various channels were noted. A power law is frequently used as the rheological model [2, 3]. However, the power-law model for a pseudo-plastic medium has a substantial drawback: at low rates of shear (shear stresses), this model yields infinitely high viscosity. In this connection, the Ellis rheological model is preferred [1]. For flow in a plane channel (Fig. 1), this model is of the form

$$\frac{\partial v_x}{\partial y} = \frac{1}{\mu}\left(1 + k|\tau_{xy}|^{m-1}\right)\tau_{xy} , \tag{1}$$

where k and m are the constants. At high rates (stresses) of shear, model (1) represents the power law, and at very low rates (stresses), describes the Newtonian behavior of a fluid. In [4], calculations of flow and heat transfer for the power law and the Ellis model were compared. It has been noted that the power-law model yields a greater error in the prediction of the fields of temperature and velocity, and also of stresses on the wall. An analysis of the literature has shown the absence of works on describing the Ellis fluid flow under nonisothermal conditions with a variable viscosity dependent on temperature and pressure. Therefore, in the present work, consideration is given to the flow of a high-viscosity non-Newtonian medium in a plane channel (Fig. 1) with variable viscosity.

Wall layers of the fluid flow in the channel are most intensely heated from its hot walls. In this region, the dissipative function has its maximum values. Furthermore, wall layers have the much longer residence time in the channel compared to the paraxial zone. A combination of these factors may give rise to a premature reaction of solidification of thermosetting plastics or to the vulcanization (subvulcanization) of rubber mixes. Therefore, we must take into account the fact that fluid flow in the channel is accompanied by the proceeding of chemical reactions that may strongly influence the rheoplastic properties of the fluid.

In the present work, we have made an effort to develop a model relatively simple for engineering applications that takes account of the dependence of the fluid′s viscosity on temperature, pressure, and the degree of chemical conversion.
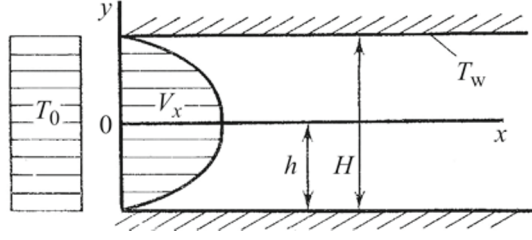
Fig. 1. Diagram of nonisothermal flow of a high-viscosity non-Newtonian medium in a plane channel.

Mathematical Model. Consideration is given to a polymer medium of high viscosity and low thermal diffusivity whose flow is implemented at small Reynolds numbers and large Péclet numbers. Therefore, a mathematical model of channel flow of such a fluid is constructed with the number of universally accepted assumptions [1]. We write the Ellis rheological equation (1) in dimensionless form

$$\frac{\partial V_x}{\partial Y} = \frac{1}{\mu} (1 + K|\sigma_{xy}|^{m-1})\sigma_{xy} , \qquad (2)$$

where $Y = y/h$, $V_x = v_x/\overline{v}_x$, $\overline{\mu} = \mu/\mu_w$, $\sigma_{xy} = \dfrac{\tau_{xy} h}{\mu_w \overline{v}_x}$, and $K = \dfrac{k \mu_w^{m-1} \overline{v}_x^{m-1}}{h^{m-1}}$.

Equation (2) is supplemented with the equation of motion in dimensionless form

$$\frac{\partial \sigma_{xy}}{\partial Y} = \frac{dP}{dX} \qquad (3)$$

and with the condition of constancy of the fluid flow rate

$$\int_0^1 V_x \, dY = 1 , \qquad (4)$$

where $P = \dfrac{ph}{\mu_w \overline{v}_x}$ and $X = x/h$.

We set the following boundary conditions:

$$Y = 0: \quad \frac{\partial V_x}{\partial Y} = 0 , \quad \frac{\partial \theta}{\partial Y} = 0 , \qquad (5)$$

$$Y = 1: \quad V_x = V_s , \quad \theta = 0 , \qquad (6)$$

$$X = 0: \quad \theta = 1 , \qquad (7)$$

where $\theta = \dfrac{T_w - T}{T_w - T_0}$.

Upon integrating (3) doubly with account of (2) and of boundary condition (6), we obtain an expression for the velocity profile in explicit form [1]:

$$V_x = V_s - \frac{dP}{dX} \int_Y^1 \frac{Y}{\overline{\mu}} \, dY + K \left(-\frac{dP}{dX} \right)^m \int_Y^1 \frac{Y^m}{\overline{\mu}} \, dY . \qquad (8)$$

We find the unknown pressure gradient, using the condition of constancy of the fluid flow rate (4)

$$-\frac{dP}{dX} \int_0^1 F_1(X, Y) \, dY + K \left(-\frac{dP}{dX} \right)^m \int_0^1 F_2(X, Y) \, dY = 1 - V_s , \qquad (9)$$

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where $F_1(X, Y) = \int\limits_Y^1 \dfrac{Y}{\overline{\mu}}\, dY$ and $F_2(X, Y) = \int\limits_Y^1 \dfrac{Y^m}{\overline{\mu}}\, dY$.

For the nonisothermal case, the hydrodynamic problem is solved simultaneously with finding the temperature field. The energy equation with account of dissipation is of the form

$$V_x \frac{\partial \theta}{\partial X} = \frac{1}{\mathrm{Pe}} \frac{\partial^2 \theta}{\partial Y^2} + \frac{\mathrm{Br}}{\mathrm{Pe}} \sigma_{xy} \frac{\partial V_x}{\partial Y}, \tag{10}$$

where $\mathrm{Pe} = \dfrac{\overline{v}_x h}{a}$ and $\mathrm{Br} = \dfrac{\mu_w \overline{v}_x^2}{\lambda(T_w - T_0)}$.

We take into account the fact that in the process of fluid flow in the channel, there is the chemical reaction which may strongly affect its rheological properties. Taking account of the dependence of the viscosity of the fluid on the degree of its conversion can fundamentally alter the entire hydrodynamic and thermal situation in the channel. Therefore, the formulated problem is solved for a polymer, whose viscosity depends on its temperature, pressure, and degree of conversion [5, 6]:

$$\overline{\mu} = \exp\left[\psi\theta + b_2 P + \frac{b_3 \beta}{\beta_* - \beta}\right], \tag{11}$$

where $\psi = b_1(T_0 - T_w)$, b_1, b_2, and b_3 are the empirical rheological constants. It is clear from (11) that the viscosity of the polymer monotonically grows and tends to infinity at $\beta \to \beta_*$. Therefore, there is no well-defined boundary between its solid and fluid phases.

Taking account of dependence (11) requires that the kinetic equation of chemical reaction be introduced in the mathematical model. It is believed that the chemical reaction is single-stage and may be described using one parameter: the degree of conversion

$$V_x \frac{\partial \beta}{\partial X} = \mathrm{Da}(a - \beta)^r \exp\left(-\frac{\overline{U}}{\theta + \gamma}\right), \tag{12}$$

where $\mathrm{Da} = \dfrac{k_0 h}{\overline{v}_x}$, $\overline{U} = \dfrac{U}{R(T_0 - T_w)}$, and $\gamma = \dfrac{T_w}{R(T_0 - T_w)}$. Equation (12) in many cases reflects the actual picture of the process and enables us to abandon complex multiparametric systems of kinetic equations. It has been shown in [7, 8] that many reactions of solidification of thermosetting plastics or vulcanization of rubber mixes are single-stage. Here, most of the grades of rubber mixes have the reaction order $r = 1.0$–1.6. Also, Eq. (12) describes the reaction of solidification of phenol-formaldehyde resins with a reaction order $r = 1.42$, and in the reactions of formation of polyurethanes, with $r = 2$ as a rule. In various works, Eq. (12) was also used to describe the kinetics of solidification of epoxy resins.

The formulated problem was solved by the iterative scheme numerically by the finite-difference method [1], with the slip velocity on the wall V_s being determined from the formula experimentally obtained in [9] and used in the mathematical model [10].

Discussion of Results. It should be noted that if calculation results are analyzed in dimensionless form, these results will be of sufficient generality and will cover the broadest range of problems in engineering practice.

It follows from kinetic equation (12) that the distribution of the degree of conversion in the flow depends on three parameters: the Damköhler number, the dimensionless activation energy $\overline{U}$, and the dimensionless temperature θ which, as seen from energy equation (10), is determined by Péclet and Brinkman numbers. Upon the change in any of these parameters with the aim of determining its influence on the course of the chemical reaction, the remaining parameters will have fixed values.

In [1], we showed the influence of the Péclet number on the development of the thickness of the solidified wall layer along the channel length. At the same time, for high-viscosity polymer compounds, the role of dissipation is important. Taking account of dissipative heat releases leads to higher temperatures of the flow and hence to a faster reaction of solidification (vulcanization). This is manifested as accelerated buildup of the thickness of the solidified layer along the channel length $X_L = x/L$ as a function of the Brinkman number at fixed values of the parameters $\overline{U}$, Pe, and $\mathrm{Da}_0 = \mathrm{Da} \exp(-\overline{U})$ (Fig. 2). It should be mentioned once again that the calculation results presented in Fig. 2 have been obtained for one value of $\overline{U}$.
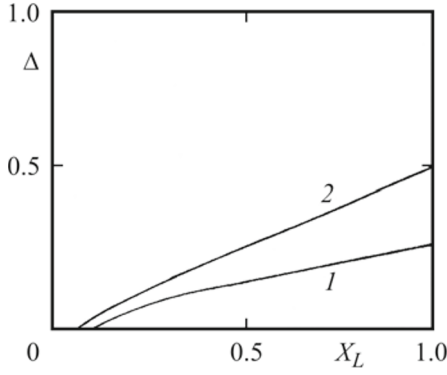
Fig. 2. Development of the thickness of a solidified layer along the channel length at $\bar{U} = 10$, Pe $= 10^3$, Da$_0 = 4$, and Br $= 0$ (1) and -10 (2).
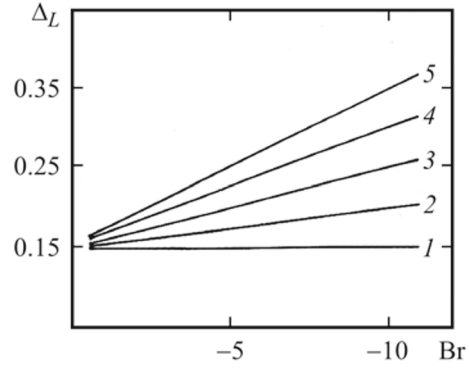
Fig. 3. Influence of the Brinkman number on the thickness of the solidified wall layer at exit from the channel at Da$_0 = 4$, Pe $= 10^4$, and $\bar{U} = 7$ (1), 17 (2), 24 (3), 30 (4), and 37 (5).
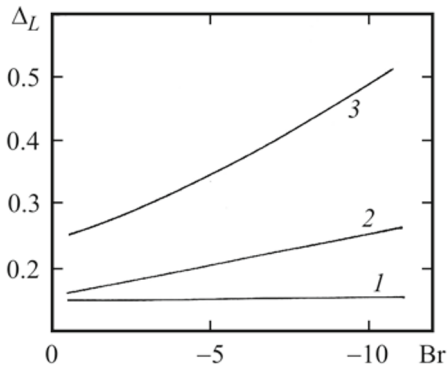

Fig. 4. Influence of the Brinkman number on the thickness of the solidified wall layer at exit from the channel Da$_0 = 4$, Pe $= 10^3$, and $\bar{U} = 1.4$ (1), 3.4 (2), and 10 (3).
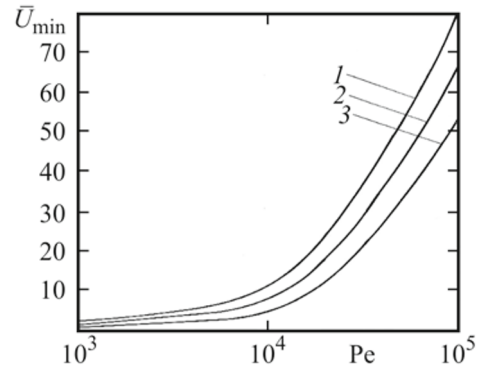
Fig. 5. Quantity $\bar{U}_{\min}$ vs. Péclet and Damköhler numbers: 1) Da$_0 = 0.5$, 2) 4, and 3) 8.

To show the degree of influence of dissipation on the course of the chemical reaction at different $\bar{U}$ values, we carried out the calculations presented in Fig. 3. The dependence of the thickness of the solidified wall layer at exit from the channel on the Brinkman number with variation of Br in a fairly wide range has been shown. The sensitivity of the chemical-reaction rate to temperature is determined by the quantity $\bar{U}$. As can be clearly seen from Fig. 3, with increase in the dimensionless activation energy $\bar{U}$, the dependence of Δ_L on Br becomes more substantial. Interestingly, $\bar{U} = 7$ is the limiting value below which Δ_L has a constant value independent of Br. This means that in the region $\bar{U} \leq 7$, the influence of dissipation on the course of the chemical reaction of solidification in the channel may be neglected. We denote the indicated limiting activation energy as $\bar{U}_{\min}$. However, this value refers only to one set of the parameters Pe and Da$_0$.

Figure 4 gives analogous results for another value of Pe; also, a new limiting value $\bar{U}_{\min} = 1.4$ has been obtained below which the value of the Br number affects no longer the thickness of the solidified layer. Carrying out similar calculations for other values of Pe and obtaining the corresponding values of $\bar{U}_{\min}$, we can construct the plot of the function $\bar{U}_{\min} = f(\text{Pe})$ for the fixed value Da$_0 = 4$. If analogous plots are constructed for other Da$_0$ values, we obtain a series of curves presented in Fig. 5. Thus, the plots in this figure allow the answer to the question as to the role of the dissipative factor at different sets of the parameters $\bar{U}$, Pe, and Da$_0$. To each pair of Pe and Da$_0$ values, there corresponds a certain value of $\bar{U}_{\min}$. At $\bar{U} > \bar{U}_{\min}$, dissipative heat releases exert an influence on the development of the solidified wall layer.

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At $\overline{U} \leq \overline{U}_{\min}$, it may be assumed that dissipation does not exert any influence on the distribution of the degree of conversion in the channel $\beta(x, y)$.

Conclusions. We are the first to formulate and solve the problem on nonisothermal flow of a non-Newtonian chemically reactive polymer medium in a plane channel on the basis of the Ellis rheological model with account taken of the dissipative heat release in the channel, and also of the dependence of the viscosity of the fluid on the temperature, pressure, and degree of its chemical conversion. The presented model is relatively simple for engineering applications in engineering practice. We have shown the substantial influence of various dimensionless parameters on the formation and rate of buildup of a solidified wall layer in fluid flow in the channel, which leads to a substantial transformation of the flow-velocity profile. The regions of fluid flow have been indicated, where the influence of dissipation on the course of the chemical reaction may be neglected.

NOTATION

a, thermal diffusivity; Da, Pe, Nu, and Br, Damköhler, Péclet, Nusselt, and Brinkman numbers; h and L, half-width of the channel and its length; p, pressure; R, universal gas constant; T, polymer temperature; T_{m}, mass mean temperature of the medium in a given cross section of the channel; T_{w}, temperature of the channel wall; T_0, polymer temperature at entry into the channel; U, activation energy of the chemical reaction; v_x, axial flow-velocity component; $\overline{v}_x$, average flow velocity; x and y, longitudinal and transverse coordinates; α, heat-transfer coefficient on the channel wall; β, dimensionless (relative) degree of chemical conversion; β_*, conversion degree at which the compound loses fluidity; Δ, thickness of the solidified wall layer at exit from the channel; λ, thermal conductivity; μ, polymer viscosity; μ_{w}, viscosity at the temperature T_{w}; τ_{xy}, shear stress. Subscripts: m, mean; min, minimum; s, shear; w, wall.

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