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THERMAL BURST IN THE FLOW OF NONLINEARLY VISCOUS MEDIA THROUGH A ROUND TUBE

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The problem of critical thermal conditions in a structurally viscous liquid flowing through an infinite tube is solved numerically with an allowance for the combined action of chemical and mechanical heat sources.

The thermal burst occurring during an exothermic chemical reaction in a medium at rest, which is characterized by a progressive temperature rise, was predicted and described in [1]. It has been shown in [2-4] that a phenomenon similar to a thermal burst can occur in the flow of a chemically inert, "exponential" liquid in an infinite tube or the flow of reactive Newtonian media whose viscosity is heavily dependent on the temperature.

We shall investigate the thermal burst in the laminar, axisymmetric flow of a generalized, structurally viscous, incompressible, and reactive liquid with an allowance for the combined action of chemical and dissipative heat release.

We assume that the thermophysical characteristics of the liquid are constant, a zero-order reaction is in progress, and a constant temperature is maintained at the tube wall. Then, the system of equations of motion and energy conservation with an allowance for dissipative heat release and heat release due to the chemical reaction has the following form:

$$\frac{\partial\tau}{\partial r}+\frac{\tau}{r}=\frac{\partial P}{\partial z}=\text{const},\ r\in(0,\ r_1),\tag{1}$$

$$\lambda\left(\frac{\partial^2T}{\partial r^2}+\frac{1}{r}\,\frac{\partial T}{\partial r}\right)+\tau\frac{\partial v}{\partial r}+Q_0k_0\exp\left(\frac{-E}{RT}\right)=0,\ r\in(0,\ r_1)\tag{2}$$

with the boundary conditions

$$\text{for}\ \ r=0\ \ \tau=0,\ \partial T/\partial r=0,\tag{3}$$

$$\text{for}\ \ r=r_1\ \ v=0,\ T=T_0=\text{const}.\tag{4}$$

As a rheological model, we shall use the Kutateladze–Khabakhpasheva equation [5] for a structurally viscous liquid,

$$\varphi_*=\exp(-\tau_*),\tag{5}$$

where $\varphi_*=(\varphi_\infty-\varphi)/(\varphi_\infty-\varphi_0)$ and $\tau_*=\Theta|\tau-\tau_0|/(\varphi_\infty-\varphi_0)$.

Since viscosity is a more complex function of the shearing stress than fluidity, which is the inverse quantity [5], the phenomenological theory of liquid flow with structural viscosity has been developed with respect to $\varphi(\tau)$, which is, for $\tau > \tau_0$, defined in the one-dimensional case as

$$dv/dr=-\varphi(\tau-\tau_0),\ r\in(r_0,\ r_1).\tag{6}$$

We represent the temperature relationships of the rheological model parameters in the Arrhenius form:

$$\varphi_0=A_0\exp(-B/RT),\ \varphi_\infty=A_\infty\exp(-B/RT),\tag{7}$$
$$\Theta=\Theta_0\exp(-B/RT),\ \tau_0=a_0\exp(-b_0(T-T_0)).$$

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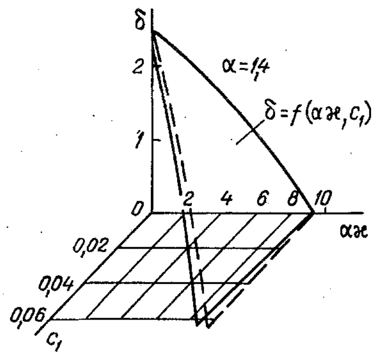

Fig. 1. Critical surface which separates the pre-burst region from the region of thermal burst (the solid curve pertains to a pseudoplastic liquid, while the dashed curve pertains to a dilating liquid).

Substituting (7) in Eq. (6) and reducing it to the dimensionless form, we obtain

$$\frac{dw}{dx} = -\frac{1}{2}\{c_0 - (c_0 - 1)\exp[-c_1(x - c_2\exp(-\beta_1\beta\theta(x_0)))]\} \times$$
$$\times [x - c_2\exp(-\beta_1\beta\theta(x_0))]\exp\left(\frac{\alpha\theta}{1+\beta\theta}\right), \quad x \in (x_0,\ 1). \tag{8}$$

Treating the equation of energy conservation in a similar manner and eliminating the shear velocity, we find

$$\frac{d^2\theta}{dx^2} + \frac{1}{x}\frac{\partial\theta}{dx} + \varkappa x\{c_0 - (c_0 - 1)\exp[-c_1(x - c_2\exp(-\beta_1\beta\theta(x_0)))]\} \times$$
$$\times [x - c_2\exp(-\beta_1\beta\theta(x_0))]\exp\left(\frac{\alpha\theta}{1+\beta\theta}\right) + \delta\exp\left(\frac{\theta}{1+\beta\theta}\right) = 0, \ x \in (x_0,\ 1). \tag{9}$$

The following notation of the dimensionless variables and parameters is used in (8) and (9).

$$w = \frac{\exp(B/RT_0)}{br_1^2A_0}v, \quad \theta = \frac{E}{RT_0^2}(T - T_0), \quad x = \frac{r}{r_1}, \quad x_0 = \frac{r_0}{r_1},$$
$$\beta = RT_0/E, \ \alpha = B/E, \ c_0 = A_\infty/A_0, \ \beta_1 = b_0T_0,$$
$$c_1 = \frac{\theta_0 br_1}{2(A_\infty - A_0)}, \quad \varkappa = \frac{b^2r_1^4A_0E}{4\lambda RT_0^2}\exp\left(\frac{-B}{RT_0}\right),$$
$$c_2 = \frac{2a_0}{br_1}, \quad \delta = \frac{Q_0k_0r_1^2E}{\lambda RT_0^2}\exp\left(\frac{-E}{RT_0}\right).$$

The parameter $\varkappa$ characterizes the intensity of the heat release due to viscous friction, δ is the Frank-Kamenetskii parameter, known from the thermal burst theory, which characterizes the intensity of heat release due to the chemical reaction, c_0, c_1, c_2, and β_1 are the parameters accounting for the rheological characteristics of the structurally viscous medium, and α is the ratio of the activation energy of viscous friction to the activation energy of the chemical reaction.

Since Eqs. (8) and (9) also describe generally the flow of a medium characterized by a yield point, the equations of motion and energy conservation break up to fit two regions: that of a quasisolid flow core $x \in (0, x_0)$, which is characterized by a constant velocity, and the shear flow region $x \in (x_0, 1)$.

For the quasisolid core region, which has no velocity gradient and, thus, no viscous friction, the equation of energy conservation assumes the following form:

$$\frac{d^2\theta_1}{dx^2} + \frac{1}{x}\frac{d\theta_1}{dx} + \delta\exp\left(\frac{\theta_1}{1+\beta\theta_1}\right) = 0, \quad x \in (0,\ x_0), \tag{10}$$

where θ_1 is the temperature of the flow core.

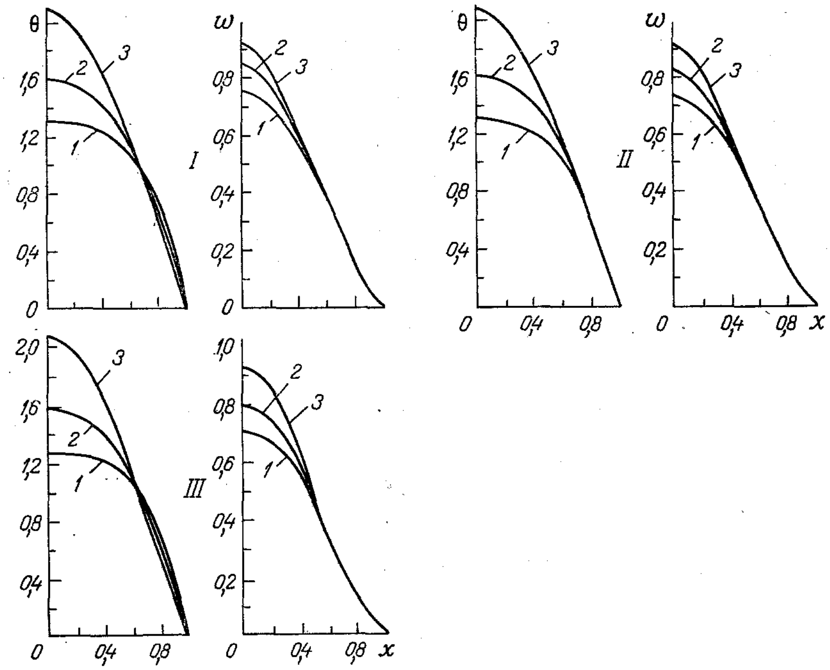

Fig. 2. Pre-burst profiles of the dimensionless temperatures θ and the velocities w for a pseudoplastic liquid 1, a Newtonian liquid 2, and a dilating liquid 3. The curves 1, 2, and 3 correspond to the following values of the Frank-Kamenetskii parameter δ: 0, 1, and 2.46, respectively.

For the shear flow region, the equations of motion and energy conservation are given by (8) and (9).

The presence of a quasisolid core involves coupling conditions at its boundary, and, therefore, the boundary conditions for Eqs. (8), (9), and (10) are the following:

$$\begin{gathered}\text{for} \quad x=0 \quad d\theta_1/dx=0,\\ \text{for} \quad x=x_0 \quad dw/dx=0,\ \theta_1=\theta,\ d\theta_1/dx=d\theta/dx,\\ \text{for} \quad x=1 \quad w=0,\ \theta=0.\end{gathered} \tag{11}$$

Although Eq. (9) does not coincide entirely with the thermal burst equation [1] and cannot be reduced to the latter by the substitution of variables, the presence of an exponential heat source nevertheless suggests that Eq. (9) with the boundary conditions (11) is qualitatively similar to the thermal burst equation. Thus, with certain conditions imposed on the parameters $\varkappa$, c_0, c_1, c_2, β_1, and δ of Eq. (9), high-density energy causing unsteady temperature and flow velocity distributions can arise within the volume of a moving structurally viscous medium. This is supported by a numerical investigation, the results of which are given below.

It is known from thermal burst theory that the existence and the number of solutions depends on the parameters characterizing the process, which are $\varkappa$, c_0, c_1, c_2, β_1, and δ in our case. If the values of these parameters are lower than the critical values, Eq. (9) has two solutions, one of which is stable, realizable in physical experiments, and characterized by a low-temperature profile. If these parameters exceed certain critical values, Eq. (9) does not have a solution, and steady-state temperature and velocity distributions are impossible. Under such conditions, the heat released as a result of viscous friction and the chemical reaction is not removed through the tube wall, which produces a temperature rise in the flow, i.e., a phenomenon referred to as thermal burst.

Thus, there exists a hypersurface in the space R^6 (where 6 is the number of the characteristic parameters $\varkappa$, c_0, c_1, c_2, β_1, and δ) which separates the region of parameters with steady-state temperature and velocity distributions from the thermal burst region.

It should also be mentioned that Eq. (10), written for the flow core, coincides exactly with the thermal burst equation [1].

We shall subsequently consider the flow of a structurally viscous liquid without a yield point, when the core region degenerates, $a_0 = 0$, and, thus, $c_2 = 0$, while the equations of motion and energy conservation (8) and (9) assume the following form:

$$\frac{dw}{dx} = -\frac{1}{2} x [c_0 - (c_0 - 1)\exp(-c_1 x)] \exp\left(\frac{\alpha\theta}{1+\beta\theta}\right), \quad x \in (0,\ 1), \tag{12}$$

$$\frac{d^2\theta}{dx^2} + \frac{1}{x}\frac{d\theta}{dx} + \varkappa x^2 [c_0 - (c_0 - 1)\exp(-c_1 x)] \exp\left(\frac{\alpha\theta}{1+\beta\theta}\right) + \delta \exp\left(\frac{\theta}{1+\beta\theta}\right) = 0, \quad x \in (0,\ 1), \tag{13}$$

with the boundary conditions

$$\text{for} \quad x = 0 \quad d\theta/dx = 0, \tag{14}$$

$$\text{for} \quad x = 1 \quad w = 0,\ \theta = 0. \tag{15}$$

The equation of energy conservation (13) can be integrated for the boundary conditions (14) and (15) independently of the equation of motion (12).

There is no known analytical solution of Eq. (13). Therefore the problem consists in solving numerically Eq. (13) and finding the dependence $\delta = f(\alpha\varkappa, c_0, c_1)$, i.e., the hypersurface in R^4 which, as was mentioned above, separates the steady-state distributions of the temperature and velocity fields from the thermal burst region.

The algorithm of numerical solution of the nonlinear equation (15) is based on the iteration principle [6], and a difference scheme with second-order approximation [7] is applied to problem (13).

Calculations were performed for problem (12), (13) with boundary conditions (14), (15) for the flow of a reactive, structurally viscous medium, using $\alpha = 1.4$, $\beta = 0.1567$, and $c_0 = 3$ for a pseudoplastic liquid and $c_0 = 0.4$ for a dilating liquid.

The calculation results were used for plotting the critical surface $\delta = f(\alpha\kappa, c_1)$ (Fig. 1), which separates the region of steady-state θ and w distributions from the thermal burst region.

For $\varkappa = 0$, i.e., in the absence of dissipative heat release, the surface degenerates into the point $\delta_{cr} \approx 2.46$. We shall subsequently omit the subscript cr, and the parameters δ, $\alpha\varkappa$, and c_1 and the dimensionless variables θ and w will denote the critical values. For $\delta = 0$, i.e., in the absence of a chemical heat source, the surface degenerates into a curve in the $(\alpha\varkappa, c_1)$ plane. For the flow of a chemically reactive Newtonian liquid in the tube (i.e., when $\theta_0 = 0$), we have $c_1 = 0$, and the surface degenerates into the $\delta = f(\alpha\varkappa)$ curve in a plane whose axes are δ and $\alpha\varkappa$.

The surface corresponding to a pseudoplastic liquid (solid curve) is located below the surface corresponding to the dilating liquid (dashed curve). This indicates that the thermal burst occurs earlier for the pseudoplastic liquid than for the Newtonian and dilating liquids.

As an example, we performed calculations for the flow of a reactive, structurally viscous system with the following parameters: for the pseudoplastic liquid, B = 26.6 kJ/mole; E = 18.72 kJ/mole; Q_0 = 54.6 kJ/mole; k_0 = 0.68 kmole/(m^3·sec); λ = 0.457 W/(m·deg K); A_0 = $26.7 \cdot 10^3$ (Pa·sec)$^{-1}$; A_∞ = $80.1 \cdot 10^{3}$ (Pa·sec)$^{-1}$; for the dilating liquid, A_∞ = $10.68 \cdot 10^3$ (Pa × sec)$^{-1}$.

For this case and a purely hydrodynamic thermal burst, the difference between the critical parameter values $\alpha\varkappa \approx 8.88$ for the pseudoplastic and $\alpha\varkappa \approx 9.51$ for the dilating liquid on the one hand and the critical parameter value $\alpha\varkappa \approx 9.18$ for the Newtonian liquid amounts to 3.5%; it increases with the absolute value of the c_1 parameter.

It should be borne in mind that the c_0 parameter also affects the critical value of $\alpha\varkappa$ for a structurally viscous liquid. With an increase in c_0, the value of $\alpha\varkappa$ decreases.

Figure 2 shows the results obtained in calculating θ and the velocities w.

Let us discuss the basic results of the numerical investigation.

1. For the case of a purely hydrodynamic thermal burst ($\delta = 0$; curves 1 in Fig. 2) in the absence of a chemical heat source, we obtained the following critical values of the parameters and the variables:

a) for a pseudoplastic liquid, $\alpha\varkappa \approx 8.88$; $c_1 \approx 0.053$; $\theta \approx 1.286$; $w \approx 0.76$, where θ is the maximum pre-burst heating, i.e., the temperature at the tube axis immediately preceding the thermal burst, and w is the maximum pre-burst velocity;
b) for a Newtonian liquid ($c_1 = 0$), $\alpha\varkappa \approx 9.18$; $\theta \approx 1{,}273$; $w \approx 0.73$;
c) for a dilating liquid, $\alpha\varkappa \approx 9.51$; $c_1 \approx 0.055$; $\theta \approx 1.260$; $w \approx 0.70$.

2. For the case of thermal burst under the combined action of chemical and dissipative heat sources ($\delta = 1$; curves 2 in Fig. 2), the critical values of the parameters and the variables are equal to:

a) for a pseudoplastic liquid, $\alpha\varkappa \approx 5.52$; $c_1 \approx 0.042$; $\theta \approx 1.610$; $w \approx 0.84$;
b) for a Newtonian liquid ($c_1 = 0$), $\alpha\varkappa \approx 5.66$; $\theta \approx 1.605$; $w \approx 0.82$;
c) for a dilating liquid, $\alpha\varkappa \approx 5.81$; $c_1 \approx 0.043$; $\theta \approx 1.588$; $w \approx 0.79$.

3. The conditions for a purely chemical thermal burst obtain for $\delta \approx 2.46$. Since there is no liquid motion ($\alpha\varkappa = 0$), the difference between the liquids is eliminated, and curves 3 in Fig. 2 are identical. This set of conditions was investigated in [1].

Our numerical analysis has shown that the maximum pre-burst temperature and velocity values decrease as the liquid properties change in passing from a pseudoplastic to a dilating liquid.

It is evident from Fig. 2 that the maximum pre-burst heating decreases (for $\alpha > 1$) as the heat source due to viscous friction becomes stronger. In the case of a hydrodynamic thermal burst, the temperature diagram is less steep at the tube axis in comparison with that for a chemical thermal burst, since the intensity of a chemical heat source is highest at the tube axis, while the intensity of a mechanical heat source is highest at the tube walls. All this is in qualitative agreement with the results obtained in [2].

NOTATION

r and z, present coordinates; r_1, tube radius; r_0, coordinates of the boundary of the flow core; $b = -\partial P/\partial z$, pressure gradient; v and T, flow velocity and temperature, respectively; T_0, temperature of the tube wall; τ, shearing stress; τ_0, yield point; φ, fluidity of a non-Newtonian liquid; φ_0 and φ_∞, fluidity for $\tau \to 0$ and $\tau \to \infty$, respectively; θ, structural stability coefficient of the liquid; k_0, θ_0, α_0, A_0, A_∞, preexponential factors; B and E, activation energy of viscous flow and of the chemical reaction, respectively; Q_0, thermal reaction effect; λ, thermal conductivity coefficient; R, universal gas constant.

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