THERMAL EXPLOSION DURING THE FLOW OF A VISCOUS LIQUID

S. A. Bostandzhiyan, A G. Merzhanov, and N. M. Pruchkina

Zhurnal Prikladnoi Mekhaniki i Teknicheskoi Fiziki, Vol. 9, No. 5, pp. 38-43, 1968

Frank-Kamenetskii has discussed a steady-state formulation of thermal explosions [1]. Bostandzhiyan et al. [2] and Bostandzhiyan and Chernyaeva [3] have shown, for the flow in a cylindrical tube of Newtonian and non-Newtonian liquids having a strong (nonlinear) temperature dependence of the viscosity, that a phenomenon analogous to thermal explosion may occur during the flow of a chemically inert liquid. Bostandzhiyan et al. [4] have also studied Couette flow and the flow between two rotating circular cylinders of a Newtonian liquid having the same temperature dependence for its viscosity. It was shown that, although the heat balance equation reduces to the equations of the steady-state theory of thermal explosion for the corresponding region, hydrodynamic thermal "explosion" was not observed in these cases. This phenomenon was found to be characteristic of only pressurized flows.

Below, we study thermal explosions during the Poiseuille flow of a viscous, chemically reactive liquid in an infinite circular cylindrical tube, and during the motion of the liquid between infinite rotating cylinders. The combined effect of chemical and mechanical heat cources are considered.

1. Flow in an infinite circular tube. We consider the axisymmetric laminar flow of a reactive, viscous, and incompressible liquid in an infinite circular tube of radius r_0 on whose surface a constant temperature T_0 is maintained. The flow occurs under the influence of a constant pressure gradient; the liquid density is constant; the reaction is of zeroth order. We assume that the dynamical viscosity has an exponential temperature dependence:

$$\mu(T) = \mu_0 \exp U/RT, \tag{1.1}$$

where μ_0 and U are constants, R is the gas constant, and T is the absolute temperature.

The transient system of equations of motion and the heat balance equation can be written, with an account of energy dissipation and heat evolution from the chemical reaction, as

$$\rho \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}\left(\mu r \frac{\partial v}{\partial r}\right),$$

$$c\rho \frac{\partial T}{\partial t} = \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) + \frac{\mu}{J}\left(\frac{\partial v}{\partial r}\right)^2 + Qk_0 \exp\frac{-E}{RT}. \tag{1.2}$$

Here v is the velocity, ρ is the density, and λ is the thermal thermal conductivity of the liquid; J is the mechanical equivalent of heat; Q is the reaction energy; k_0 is the preexponential factor; and E is the activation energy.

We assume that the liquid temperature is initially equal to the temperature of the tube walls and that the velocity profile corresponds to isothermal flow, that is [5],

$$T(r) = T_0, \quad v(r) = \frac{br_0^2}{4\mu(T_0)}\left(1 - \frac{r^2}{r_0^2}\right)$$

$$\text{for } t=0 \quad \left(b = -\frac{\partial p}{\partial z}\right). \tag{1.3}$$

System (1.2) must be solved with the initial conditions (1.3) and the boundary conditions

$$v = 0, \quad T = T_0 \quad \text{for } r = r_0,$$

$$\frac{\partial v}{\partial r} = 0, \quad \frac{\partial T}{\partial r} = 0 \quad \text{for } r = 0. \tag{1.4}$$

Converting (1.2)-(1.4) to dimensionless form, we find

$$\frac{1}{P}\frac{\partial w}{\partial \tau} = 1 + \frac{1}{x}\frac{\partial}{\partial x}\left[\exp\frac{-\alpha\theta}{1+\beta\theta}\, x\, \frac{\partial w}{\partial x}\right],$$

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial x^2} + \frac{1}{x}\frac{\partial \theta}{\partial x} +$$

$$+ 4\varkappa_1 \exp\frac{-\alpha\theta}{1+\beta\theta}\left(\frac{\partial w}{\partial x}\right)^2 + \delta \exp\frac{\theta}{1+\beta\theta}, \tag{1.5}$$

$$\theta(x) = 0, \quad w(x) = {}^1/_4(1 - x^2) \quad \text{for } \tau = 0,$$

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

$$\frac{\partial w}{\partial x} = 0, \quad \frac{\partial \theta}{\partial x} = 0 \quad \text{for } x = 0. \tag{1.6}$$

Here

$$w = \frac{\mu(T_0)}{br_0^2}v, \qquad \theta = \frac{E}{RT_0^2}(T - T_0),$$

$$x = \frac{r}{r_0}, \qquad \tau = \frac{\lambda}{c\rho r_0^2}t$$

are dimensionless variables, and

$$\varkappa_1 = \frac{b^2 r_0^4 E}{4J\lambda\mu(T_0)RT_0^2}, \quad \delta = \frac{QEk_0 r_0^2}{\lambda RT_0^2}\exp\frac{-E}{RT_0},$$

$$P = \frac{c\mu(T_0)}{\lambda}, \quad \beta = \frac{RT_0}{E}, \quad \alpha = \frac{U}{E}$$

are dimensionless parameters.

The parameter $\varkappa_1$ characterizes the heat-evolution rate due to internal friction, and differs from the analogous parameter $\varkappa$ of [2] by the constant factor ($\varkappa_1 = 4\varkappa/\alpha$); δ is the Frank-Kamenetskii parameter, found from thermal-explosion theory [1]; P is the Prandtl number; β is a dimensionless parameter, usually small; and α is the ratio of the activation energy for viscous flow to that of the chemical reaction.

When $P \gg 1$, the hydrodynamic-relaxation time is much smaller than the thermal-relaxation time, so, from the hydrodynamical point of view, the process is quasi-steady-state; that is, the time required for a steady state to be established is governed by the heat-conduction equation. The velocity profile is rapidly levelled off as the temperature changes. Curves showing the establishment of a steady-state temperature for various P values will be given below.

Strictly speaking, we should choose a quiescent state rather than an established velocity profile for the initial condition (1.6). However, it should be noted that the initial velocity distribution can have an effect only during the induction period; it will not affect such characteristics

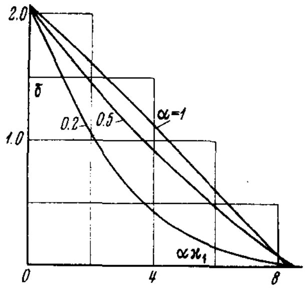

Fig. 1

of the thermal explosion as the critical condition or the preexplosion heating. When, however, P ≫ 1 (the case for which calculations are carried out here), the induction period is much longer than the hydrodynamic-relaxation time, so the initial velocity distribution does not play a significant role. Under these conditions, an established velocity profile may be adopted as the initial condition.

For a quasi-steady-state process, we may set $\partial w/\partial\tau = 0$. Integrating the first equation in system (1.5) and using the boundary condition at the tube axis, we find

$$\frac{\partial w}{\partial x} = -\frac{1}{2} x \exp\frac{\alpha\theta}{1+\beta\theta}. \qquad (1.7)$$

Using (1.7), we can eliminate the velocity gradient from the second equation in system (1.5):

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial x^2} + \frac{1}{x}\frac{\partial\theta}{\partial x} + \varkappa_1 x^2 \exp\frac{\alpha\theta}{1+\beta\theta} + \delta\exp\frac{\theta}{1+\beta\theta}. \qquad (1.8)$$

Thus, the heat balance equation can be integrated separately from the hydrodynamical equation. The temperature profile is found from Eq. (1.8) with the initial and boundary conditions (1.6). After determining θ, we find the velocity profile from (1.7).

If we set $\varkappa_1 = 0$ in Eq. (1.8) (corresponding to no mechanical heat sources), we find the problem of thermal explosion in a cylindrical region. The critical value δ_* of the Frank-Kamenetskii parameter, the maximum preexplosion heating θ_*, and the adiabatic induction period τ'_* ($\tau = \delta\tau$) are known to depend slightly on β. The following approximate equations have been found for these quantities [6,7]:

$$\delta_*(\beta) \approx \delta_*(1+\beta), \quad \theta_*(\beta) \approx \theta_*(1+2\beta),$$
$$\tau_*'(\beta) \approx \tau_*'(1+2\beta). \qquad (1.9)$$

The factors in parentheses denote the values of the corresponding quantities at $\beta = 0$ ($\delta_* = 2$, $\theta_* = 1.38$, and $\tau'_* = 1$—see [1]).

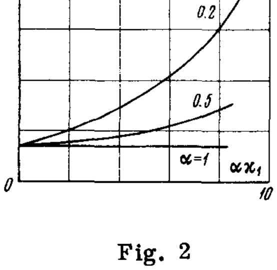

Fig. 2

Setting $\delta = 0$ in Eq. (1.8) (that is, for no chemical heat sources), we find the problem of the hydrodynamic thermal "explosion" [2]. Taking into account the difference between the dimensionless temperatures of this study and of [2], we find the following approximations for the critical parameter $\varkappa_1$ and the maximum preexplosion heating for a hydrodynamic thermal "explosion":

$$\varkappa_{1*} \approx \frac{8}{\alpha}\left(1+\frac{\beta}{\alpha}\right), \qquad \theta_* \approx \frac{1.38}{\alpha}\left(1+\frac{2\beta}{\alpha}\right). \qquad (1.10)$$

When the two types of heat sources act jointly in the critical region, there is a functional relationship between δ and $\varkappa_1$. It follows that curves plotted as dependences of δ on $\alpha\varkappa_1$ for various α values will begin at the point $\delta_*(\beta)$ on the axis of ordinates and will end at the point of $\alpha\varkappa_{1*}$ on the axis of abscissas. These curves separate the δ and $\varkappa_1$ ranges in which steady-state temperature and velocity fields are set up from those in which thermal explosion occurs.

The explicit dependence of δ on $\varkappa_1$ cannot be found, since no analytic solution is known for Eq. (1.8), even for $\beta = 0$.

Equation (1.8) was integrated numerically on a computer. All the calculations were carried out for $\beta = 0.03$. Figure 1 shows the $\delta_* = f(\alpha\varkappa_1)$ dependence for $\alpha = 1, 0.5, 0.2$. The region bounded by the coordinate axes and the curve is that in which the steady-state temperature and velocity fields are set up smoothly. If the point with coordinates δ and $\alpha\varkappa_1$ is outside this region, the steady state is not attained, and there is a thermal explosion.

Figure 2 shows for the same α values the dependences of the maximum preexplosion heating on $\alpha\varkappa_1$. Since thermal explosion occurs when $\varkappa_1 = 0$ without mechanical heat sources, and Eq. (1.8) does not contain α, all the curves begin at the same point, given approximately by Eq. (1.9). The ends of the curves correspond to the case of a hydronamic-thermal "explosion"; here the maximum "preexplosion" heating is given approximately by Eq. (1.10). For $\alpha = 1$, the preexplosion heating remains almost constant; for $\alpha < 1$, it increases, reaching its greatest value at $\delta = 0$.

Figures 3–5 show the dependences of the induction period on the parameters $\varkappa_1$, δ, and $\varkappa_1/\delta$, calculated for $\alpha = 0.5$. Figure 3 shows the dependence of the induction period on the parameter $\varkappa_1$ found for various values of the Frank-Kamenetskii parameter. The first curve was found for the case of a hydrodynamic thermal explosion; the third curve was found for the case of a thermal explosion without mechanical heat sources. For $0 < \delta < 2.07$, the induction period increases without bound as $\varkappa_1$ approaches the critical value. For $\delta > 2.07$, the induction period is bounded for all values of $\varkappa_1$, and at large values of δ, it depends very slightly on $\varkappa_1$ (an adiabatic thermal explosion occurs).

Figure 4 shows the analogous dependences of the induction period on the parameter δ, found for five values of the parameter $\varkappa_1$. The first curve shows the dependence of τ on δ during a chemical thermal explosion; the third curve shows the dependence for a hydrodynamic thermal "explosion; the third curve shows the dependence for a hydrodynamic thermal "explosion. "

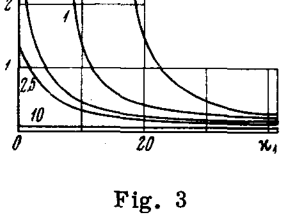

Fig. 3

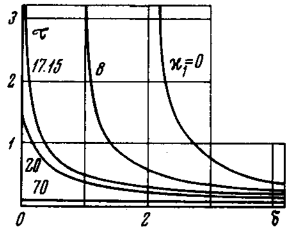

Fig. 4

Figure 5 shows, in a semilogarithmic plot, the dependences of the induction period $\tau' = \delta\tau$ on the ratio $\varkappa_1/\delta$ for five values of δ. The dimensionless time τ' differs from τ by the scale factor δ. As $\varkappa_1$ approaches the critical value for $0 < \delta < 2.07$, τ' increases without bound. When $\delta > 2.07$, τ' is bounded for all $\varkappa_1$ values; it falls off with increasing δ, and, at small $\varkappa_1$, tends toward the adiabatic induction period given approximately by Eq. (1.9). Figure 5 shows that the $\delta = 5$ and $\delta = 10$ curves characterize an adiabatic thermal explosion. At small $\varkappa_1/\delta$ values such that the effects of the mechanical heat sources are negligible, the induction periods tend toward a constant value. As $\varkappa_1$ increases, the contribution of mechanical heat sources increases, and the induction period decreases.

We briefly consider the applicability of the quasi-steady-state equation (1.8). For determining such characteristics of a thermal explosion as the critical condition and the preexplosion heating, Eq. (1.8) is valid for all values of the Prandtl number—both large and small. In fact, the critical values of the parameters are found from the condition for the absence of a steady-state solution of system (1.5), and the steady-state solutions of this system and of the quasi-steady-state equation (1.8) are the same. The Prandtl number has an effect on the temporal characteristics of the thermal explosion, i.e., on the induction period and the time before steady state is reached. From Eqs. (1.5) and (1.8), we see that the difference between the temperature profiles found from the non-steady-state solution of the equations and from the quasi-steady-state equation decreases with decreasing $\varkappa_1$, and disappears at $\varkappa_1 = 0$. The greatest difference between the solutions of system (1.5) and Eq. (1.8) for a given P is found at $\delta = 0$ and for maximum $\varkappa_1$, i.e., during a hydrodynamic thermal explosion. Special calculations were made on the basis of system (1.5) and the quasi-steady-state equation (1.8) for $\delta = 0$, $\alpha = 0.5$, $\beta = 0.03$, and four values of the Prandtl number (P = 1, 10, 100, and 1000) to evaluate the effect of the latter on the critical conditions and the time required to reach steady state. As expected, the critical value $\varkappa_{1_*} = 17.15$ and the maximum preexplosion heating $\theta_* = 3.16$ were independent of P and were the same as the values given by the quasi-steady-state equation. Time dependences of the temperature at the cylinder axis were plotted near critical conditions, below the explosion limit, for $\varkappa = 17$ (Fig. 6). Curve 1 was plotted for P = 1, and curve 2 for P = 10. The curves for P = 100 and 1000 essentially coincide with that found from the quasi-steady-state equation (curve 3). Figure 6 shows that, even at P = 10, the quasi-steady-state equation gives a solution differing little from the non-steady-state solution.

2. Flow between two rotating cylinders. We assume a viscous, chemically reactive liquid between two infinite coaxial cylinders. The inner cylinder is fixed, and the outer is rotating at a constant angular velocity ω_0. The radii and temperatures of the cylinders are r_1, r_0, T_1, and T_0. The temperature dependence of the viscosity is given by Eq. (1.1).

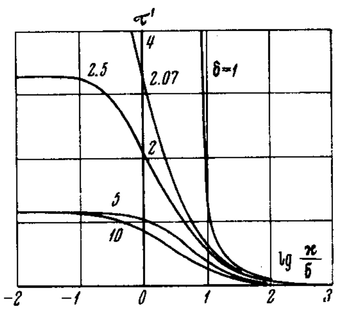

Fig. 5

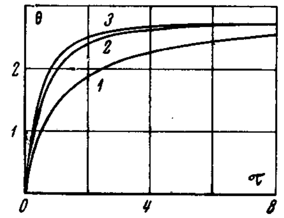

Fig. 6

The system of equations of motion and the heat balance equation can be written, with account for energy dissipation and the chemical reaction, as

$$\frac{\partial\omega}{\partial t} = \frac{1}{\rho r^3}\frac{\partial}{\partial r}\left(\mu r^3\frac{\partial\omega}{\partial r}\right),$$

$$c\rho\,\frac{\partial T}{\partial t} = \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) + \frac{\mu}{J}\left(r\frac{\partial\omega}{\partial r}\right)^2 + Qk_0\exp\frac{-E}{RT}, \qquad (2.1)$$

where ω is the angular rotation velocity of the liquid particles; the rest of the notation is the same as in Section 1.

We assume the liquid temperature is initially equal to that of the outer cylinder, and that the angular-velocity profile corresponds to isothermal flow; i.e. [5],

$$T(r) = T_0,\quad \omega(r) = \frac{\omega_0 r_0^2}{r_0^2 - r_1^2}\left(1 - \frac{r_1^2}{r_0^2}\right)\ \text{for}\ t = 0 \qquad (2.2)$$

System (2.1) must be solved with the initial conditions (2.2) and the boundary conditions

$$\omega = 0,\quad T = T_1\ \text{for}\ r = r_1,$$
$$\omega = \omega_0,\quad T = T_0\ \text{for}\ r = r_0. \qquad (2.3)$$

Converting (2.1)–(2.3) to dimensionless form, we find

$$\frac{1}{P}\frac{\partial\Omega}{\partial\tau} = \frac{1}{x^3}\frac{\partial}{\partial x}\left[\exp\frac{-\alpha\theta}{1+\beta\theta}x^3\frac{\partial\Omega}{\partial x}\right],$$

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial x^2} + \frac{1}{x}\frac{\partial\theta}{\partial x} + \varkappa\exp\frac{-\alpha\theta}{1+\beta\theta}\left(x\frac{\partial\Omega}{\partial x}\right)^2 + \delta\exp\frac{\theta}{1+\beta\theta}, \qquad (2.4)$$

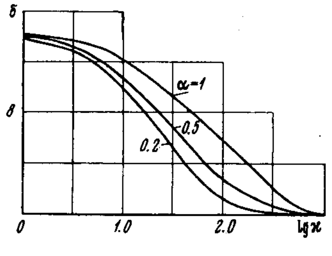

Fig. 7

$$\theta(x) = 0, \quad \Omega(x) = \frac{1}{1-d^2}\left(1 - \frac{d^2}{x^2}\right) \quad \text{for } \tau = 0,$$
$$\theta = \theta_1, \quad \Omega = 0 \quad \text{for } x = d,$$
$$\theta = 0, \quad \Omega = 1 \quad \text{for } x = 1. \qquad (2.5)$$

Here

$$\Omega = \frac{\omega}{\omega_0}, \quad \varkappa = \frac{\mu(T_0)\,\omega_0^2 r_0^2 E}{J\lambda R T_0^2},$$
$$d = \frac{r_1}{r_0}, \quad \theta_1 = \frac{E}{RT_0^2}(T_1 - T_0).$$

The rest of the notation for the dimensionless variables and parameters is the same as in Section 1.

If both cylinders are fixed ($\varkappa = 0$), the second equation in system (2.4) governs the thermal explosion of the liquid at rest between the cylinders. In this case, the critical value of the Frank-Kamenetskii parameter will depend on the ratio of radii and on θ_1. If no chemical reaction is occurring ($\delta = 0$), system (2.4) has a steady-state solution for any $\varkappa$ (as was mentioned above), and the maximum temperature will be a monotonic function of $\varkappa$. Since the dissipative heating increases monotonically with increasing $\varkappa$, then, no matter how small δ is, there is some sufficiently large $\varkappa$ which will lead to a thermal explosion. Accordingly, the $\delta(\varkappa)$ dependences will asymptotically approach the axis of abscissas for any α.

The $\delta(\varkappa)$ dependences were calculated for the following parameter values: $\beta = 0.03$; $d = 0.5$; $\theta_1 = 0$; and $\alpha = 1$, 0.5, and 0.2. The corresponding curves are shown in Fig. 7. At $\varkappa = 0$, the mass at rest between fixed cylinders will undergo a thermal explosion; here $\delta_* = 14.32$. The curves begin at this point at $-\infty$ and asymptotically approach the axis of abscissas with increasing $\varkappa$. The preexplosion heating increases monotonically with increasing $\varkappa$.

REFERENCES

1. D. A. Frank-Kamenetskii, Heat Transfer and Diffusion in Chemical Kinetics [in Russian], Izd-vo AN SSSR, 1947.

2. S. A. Bostandzhiyan, A. G. Merzhanov, and S. I. Khudyaev, "Hydrodynamic thermal explosion," Dokl. AN SSSR, **163**, no. 1, 1965.

3. S. A. Bostandzhiyan, M. Chernyaeva, and S. S. M. Chernyaeva, "Hydrodynamic thermal 'explosion' of a Newtonian liquid," Dokl. AN SSSR, **170**, no. 2, 1966.

4. S. A. Bostandzhiyan, A. G. Merzhanov, and S. I. Khudyaev, "Some problems in the nonisothermal steady-state flow of a viscous liquid," PMTF [Journal of Applied Mechanics and Technical Physics], no. 5, 1965.

5. S. M. Targ, Fundamental Problems of the Theory of Laminar Flow [in Russian], Gostekhizdat, Moscos-Leningrad, 1951.

6. A. G. Merzhanov and F. I. Dubovitskii, "Current state of the theory of thermal explosion," Usp. khimii, **35**, no. 4, 1966.

7. V. V. Barzykin, V. T. Gontkovskaya, A. G. Merzhanov, and S. I. Khudyaev, "Non-steady-state theory of thermal explosion," PMTF, no. 3, 1964.

22 January 1967 Moscow