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# A CONJUGATE PROBLEM OF THERMAL EXPLOSION OF A HOLLOW CYLINDER

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*A conjugated problem of heat conduction for two hollow cylinders that are in close contact, with one consisting of a reagent, has been solved analytically. The problem has been solved by the backward method under boundary conditions of the first kind. The critical conditions of thermal explosion were investigated as functions of the parameters of a reagent and of an inert body. An engineering method for determining the critical conditions of a thermal explosion is suggested.*

The development and application to practice of explosives culminate successively only on condition that their technological safety is ensured. This fact has stimulated the emergence of a large number of scientific studies aimed at solving various problems of technological safety. The sensitivity of explosive systems to heat characterizes their safety in the process of production. The results of studies of the thermal sensitivity of reagents carried out for years were generalized in reviews such as, for example, [1].

In the majority of cases, an explosive chemical reaction is initiated in the apparatuses that process explosives. In view of this, in modeling the problems of technological safety, it is necessary to take into account the influence of the inert walls of an apparatus or of its elements on the thermal processes proceeding in the reagents. Such an account can be taken in solving a conjugate problem of heat conduction. For a plane reagent, such a problem under boundary conditions of the first, second, and third kinds was considered in [2–4].

In the present work, we consider a thermal explosion of a reagent in the form of a hollow cylinder that is in close contact with another inert hollow cylinder.

The statement of the problem amounts to the following: there is a system consisting of two infinite hollow cylinders, where one cylinder is located inside the other. The outer hollow cylinder with outer and inner radii $R_2$ and $R_1$ consists of an inert material. The inner cylinder consists of a condensed explosive, and it is limited to the radii $R_0$ and $R_1$. The side surfaces of the cylinders at $r = R_1$ are in close contact with each other. On the surfaces of the cylinders having radii $R_0$ and $R_2$, constant temperatures $T_0$ and $T_2$, respectively, are maintained. We consider the case where $T_0 > T_2$. In the condensed explosive, an exothermal reaction of zero order proceeds, the rate of which is described by the Arrhenius equation. The volumetric power of heat release as a result of the chemical reaction is defined by the expression $q_v = Q_v K_0 \exp[-E/(RT)]$. On the surface where the explosive is adjacent to the inert wall there is a perfect thermal contact. The aim of this work is to investigate the critical conditions of thermal explosion of a reagent in a steady-state statement.

Introducing dimensionless variables and parameters $\theta = E(T - T_0)/(RT_0^2)$, $\theta_1 = E(T_1 - T_0)/T_0^2$, $\xi = r/H$, $V = E(U - T_0)/(RT_0^2)$, $k = R_0/R_1$, $H = R_1 - R_0$, $k_0 = k/(1 - k)$, $k_1 = 1/(1 - k)$, $k_2 = R_2/H$, $K_\lambda = \lambda_1/\lambda_2$, and $\text{Fk} = Q_v K_0 \exp[-E/(RT_0)]EH^2/(\lambda RT_0^2)$ and applying expansion of the exponent in the Arrhenius equation according to Frank-Kamenetskii [5], we can formulate the mathematical model of the problem in dimensionless form as

$$\frac{d^2\theta}{d\xi^2} + \frac{1}{\xi}\frac{d\theta}{d\xi} + \text{Fk} \exp \theta = 0 , \tag{1}$$

$$\frac{d^2V}{d\xi^2} + \frac{1}{\xi}\frac{dV}{d\xi} = 0 , \tag{2}$$

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$$\theta = 0 \quad \text{at} \quad \xi = k_0 , \tag{3}$$

$$\theta = V \quad \text{at} \quad \xi = k_1 , \tag{4}$$

$$\frac{d\theta}{d\xi} = K_\lambda \frac{dV}{d\xi} \quad \text{at} \quad \xi = k_1 , \tag{5}$$

$$V = \theta_2 \quad \text{at} \quad \xi = k_2 . \tag{6}$$

In going to dimensionless variables and parameters, the temperature on the reagent surface $T_0$ was used as the scalar one, whereas the width of the annular layer of the reagent $H = R_1 - R_0$ was taken as the characteristic dimension.

A stationary solution of Eq. (1) that satisfies the boundary conditions is possible only when $\mathrm{Fk} < \mathrm{Fk}_{cr}$; the absence of this condition is taken to be a thermal explosion [5]. Thus, the finding of the critical conditions of a thermal explosion amounts to the determination of $\mathrm{Fk}_{cr}$ by solving a system of equations (1)–(6). However, the solution of a relatively complex mathematical model of the problem does not allow one to obtain, in an explicit form, an expression to determine $\mathrm{Fk}_{cr}$.

In recent years, to solve complex boundary-value problems of heat conduction, backward methods have been used [6–8]. In contrast to straightforward methods, in which the temperature field of an object is determined, in the backward methods the values of the temperatures of an object are given on characteristic sites and the parameters or coefficients entering into the boundary conditions or into the heat-conduction equation are sought.

The system of equations (1)–(6) is solved by the backward method, that is, the value of a dimensionless temperature $\theta_1$ on the contact surface ($\xi = 1$) is assigned, and two independent problems are solved for the reagent and inert body, which are defined by the following equations:
for the reagent

$$\frac{d^2\theta}{d\xi^2} + \frac{d\theta}{\xi d\xi} + \mathrm{Fk} \exp \theta = 0 , \tag{7}$$

$$\theta = 0 \quad \text{at} \quad \xi = k_0 , \tag{8}$$

$$\theta = \theta_1 \quad \text{at} \quad \xi = k_1 , \tag{9}$$

for the inert body

$$\frac{d^2V}{d\xi^2} + \frac{dV}{\xi d\xi} = 0 , \tag{10}$$

$$V = \theta_1 \quad \text{at} \quad \xi = k_1 , \tag{11}$$

$$V = \theta_2 \quad \text{at} \quad \xi = k_2 . \tag{12}$$

By solving systems (7)–(9) the values of $\mathrm{Fk}_{cr}$ and $d\theta/d\xi$ at $\xi = k_1$ are determined and the solution of system (10–(12) yields the value of $dV/d\xi$ at $\xi = k_1$. The solutions of the two problems are conjugated by Eq. (5), from which the value of $K_\lambda$ is calculated. Computational operations are continued until the calculated value of $K_\lambda$ coincides practically with the real one.

We will investigate the problem of a thermal explosion of a reagent with the aid of the above-given system of equations (7)–(9). The solution of Eq. (7) is given in [5] in the form

$$\exp \theta = a/[\xi^2 \cosh^2 (\mu \ln \xi - b)] . \tag{13}$$

On the strength of boundary conditions (8) and (9), Eq. (13) yields

$$\cosh^2 (\mu \ln k_0 - b) = a/k_0^2 , \tag{14}$$

$$\cosh^2 (b - \mu \ln k_1) = a \exp (- \theta_1)/k_1^2 . \tag{15}$$

In Eq. (15), the evenness of the function of the hyperbolic cosine is used, $\cosh x = \cosh (-x)$. Excluding the integration constant $b$ from (14) and (15) yields an equation that relates the parameter Fk to the integration constant $a$:

$$\mu = \operatorname{arcosh} (a^{0.5}/k_0) + \operatorname{arcosh} \left\{[a \exp (- \theta_1)]^{0.5}/k_1\right\} . \tag{16}$$

Since $\mu^2 = a\text{Fk}/2$ [5], the solution of (16) for Fk gives

$$\text{Fk} = 2 \left\{\operatorname{arcosh} (a^{0.5}/k_0) + \operatorname{arcosh} [a \exp (- \theta_1)]^{0.5}/k_1\right\}^2 /(a \ln^2 k) . \tag{17}$$

With the inverse function of the hyperbolic cosine being replaced by a logarithmic one, Eq. (17) can be written in a more compact form:

$$\text{Fk} = 2 \ln^2 (pq)/(a \ln^2 k) , \tag{18}$$

where $p = x + (x^2 - 1)^{0.5}$; $x = a^{0.5}/k_0$; $q = z + (z^2 - 1)^{0.5}$; $z = [a \exp (-\theta_1)]^{0.5}/k_1$; $\operatorname{arch} \left\{[a \exp (- \theta_1)]^{0.5}/k_1\right\} = \ln q$, and $\operatorname{arcosh} (a^{0.5}/k_0) = \ln p$.

The critical value of the parameter $\text{Fk}_{cr}$ is determined by the maximum of the right-hand side of Eq. (18) as a function of $a$ by using the iteration method.

The estimation of the correspondence of the assigned value of $\theta_1$ to its real value is made with the aid of Eq. (5), which involves the derivatives $d\theta/d\xi$ and $dV/d\xi$ at $\xi = k_1$. It is more convenient to differentiate Eq. (13) after logarithms have been preliminarily taken in it:

$$\theta = \ln a - 2 \ln \xi - 2 \ln [\cosh (b - \mu \ln \xi)] . \tag{19}$$

Differentiation of Eq. (19) at $\xi = k_1$ leads to the expression

$$d\theta/d\xi = - 2 [1 - \tanh (\ln q) \mu]/k_1 , \tag{20}$$

where it is taken into account that $b - \mu \ln k_1 = \ln q$.

We now pass to consideration of the mathematical model of an inert body for determining $dV/d\xi$. The solution of Eq. (10) has the form

$$V = C_2 + C_1 \ln \xi . \tag{21}$$

Using boundary conditions (11) and (12), we obtain

$$\theta_1 = C_2 + C_1 \ln k_1 , \tag{22}$$

$$\theta_2 = C_2 + C_1 \ln k_2 . \tag{23}$$

TABLE 1. Dependence of the Critical Parameter $Fk_{cr}$ on the Coefficient $K_\lambda$

| $-\theta_1$ | $g_1/g_2$ | $K_\lambda$ | $Fk_{cr}$ |
|---|---|---|---|
| 6.4 | 0.5 | 0.5 | 41 |
| 9.5 | 1.0 | 1.0 | 81 |
| 12.3 | 2.0 | 2.0 | 130 |

Having eliminated $C_2$ from these equations, we obtain that $C_1 = (\theta_1 - \theta_2)/[\ln (k_1/k_2)]$. The differentiation of Eq. (21) at $\xi = k_1$ yields an expression for determining the temperature gradient on the surface of an inert material:

$$dV/d\xi = (\theta_1 - \theta_2)/[\ln (k_1/k_2)\, k_1] \, . \qquad (24)$$

Let, for brevity, the left-hand sides of Eqs. (20) and (24) be designated as $g_1$ and $g_2$, respectively. Then the given value of $\theta_1$ corresponds to reality if $g_1/g_2 \cong K_\lambda$.

In conclusion, we will consider the solution of the engineering problem of safety.

**Statement of the Problem.** There is a system consisting of two cylinders in close contact (a cylinder in a cylinder). The inner cylinder is a reagent, whereas the outer one consists of an inert material. It is necessary to determine the critical conditions of safety at $K_\lambda = 0.5$, 1.0, and 2.0. Let $T_0 = 430$ K, $T_2 = 300$ K, $R_0 = 0.10$ m, $R_1 = 0.15$ m, $H = 0.05$ m, $R_2 = 0.20$ m, $H_1 = 0.05$ m, and $E/R = 24{,}250$ K.

**Solution.** We calculate the values of $\theta_2 = E(T_2 - T_0)/(RT_0^2)$, $k = R_0/R_1$, $k_0 = R_0/H$, $k_1 = R_1/H$, and $k_2 = R_2/H$ from the initial data of the problem. We select $\theta_1$ using the inequality $0 < |\theta_1| < |\theta_2|$. The critical condition of safety is determined by the value of $Fk_{cr}$, which is calculated from (18) by the method of successive approximations. The selection of the variants of $\theta_1$ is over as soon as $g_1/g_2 \cong K_\lambda$. The values of $g_1$ and $g_2$ are determined from Eqs. (20) and (24). The results of the calculations are presented in Table 1, from which it is seen that the critical parameters depend substantially on $K_\lambda$. When $K_\lambda < 1$, the material of the inert cylinder, relative to the reagent, is a thermal insulator, whereas at $K_\lambda > 1$ it is a heat sink.

If a reagent is in close contact with a steel wall, the heat-conduction ratio $K_\lambda$ has a value of order 400. Therefore, in steel apparatuses that process explosives, the walls do not possess insulating properties, and the value of $T_1$ is practically equal to $T_2$.

Thus, a conjugate problem of a thermal explosion of explosives having the form of a hollow cylinder has been solved analytically by the backward method. It is shown that application of this method allows one to replace the solution of a complex conjugate problem by solutions of two independent problems for a reagent and an inert body. An engineering method of calculation is suggested for determining the critical conditions of a thermal explosion and the influence of the parameters of the reagent and inert body on the critical conditions is investigated.

## NOTATION

$C_1$ and $C_2$, integration constants in the problem for an inert body; $E$, activation energy, J/mole; $H$ and $H_1$, thicknesses of the annular layer of a reagent and inert material, m; $K_0$, pre-exponential factor, sec$^{-1}$; $Q_v$, thermal effect of reaction per unit volume, J/m$^3$; $R$, universal gas constant, J/(mole·K); $R_0$, $R_1$, and $R_2$, radii of cylinders, m; $T$, current temperature of a reagent, K; $T_0$, $T_1$, and $T_2$, temperatures of the inner, contact, and outer surfaces of cylinders, K; $U$, dimensional temperature of inert material, K; $V$, dimensionless temperature of inert material; $\theta$ and $\theta_1$, dimensionless temperatures (current one and that on a contact surface); $\lambda$ and $\lambda_1$, thermal conductivities of a reagent and inert material, W/(m·K); $\xi$, dimensionless coordinate. Subscripts: cr, critical; v, volume.

## REFERENCES


1. A. G. Merzhanov, V. V. Barzykin, and V. G. Abramov, Theory of thermal explosion, *Zh. Khim. Fiz.*, **15**, No. 6, 3–44 (1996).
2. A. K. Kolesnikov, Thermal explosion in a layer with boundaries of different temperature in a cross flow of a reagent, *Fiz. Goreniya Vzryva*, **20**, No. 3, 64–65 (1984).

3. R. Sh. Gainutdinov, Conjugate problem of thermal explosion, *Inzh.-Fiz. Zh.*, **72**, No. 2, 206–109 (1999).
4. R. Sh. Gainutdinov, Conjugate problem of a thermal explosion with boundary conditions of the second kind, *Inzh.-Fiz. Zh.*, **74**, No. 1, 103–105 (2001).
5. D. A. Frank-Kamenetskii, *Diffusion and Heat Transfer in Chemical Kinetics* [in Russian], Nauka, Moscow (1987).
6. O. M. Alifanov, *Inverse Problems of Heat Transfer* [in Russian], Mashinostroenie, Moscow (1988).
7. L. A. Kozdoba and P. G. Krukovskii, *Methods of Solution of Inverse Problems of Heat Transfer* [in Russian], Naukova Dumka, Kiev (1982).
8. R. Sh. Gainutdinov, Thermal explosion of a hollow cylinder under boundary conditions of the third kind, *Fiz. Goreniya Vzryva*, **40**, No. 2, 29–32 (2004).