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CONJUGATE PROBLEM OF THERMAL EXPLOSION

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The problem of thermal explosion of a reagent in the form a plane layer placed between two plane-parallel inert walls is solved analytically under boundary conditions of the third kind. Critical conditions for thermal explosion for the general case and particular cases are investigated. Results of calculations are compared with previously published data. An engineering method for evaluation of the critical conditions for thermal explosion is proposed.

Production of explosives is classified as an explosion-hazardous technology. Providing safe conditions for work in this industry is an involved problem that requires employment of theoretical and experimental methods. The need to provide safe conditions for explosives processing has stimulated numerous investigations of thermal explosion [1]. Problems of explosion safety have acquired even greater importance in recent years in connection with the introduction of high-energy explosives having a higher sensitivity to thermal effects compared to conventional explosives. In most cases, thermal explosions occur in explosives-processing apparatuses. Therefore, processes taking place in these cases are modeled with account for the effect of inert walls. The thermal explosion of a reagent placed between two inert walls has been investigated numerically in [2] under boundary conditions of the first kind. We made an attempt to solve this problem analytically under boundary conditions of the third kind on the outer surfaces of the inert walls. The formulation of the problem is as follows. A condensed explosive in the form of an infinite plate of thickness H and heat conduction coefficient λ is placed between two inert walls with coefficients of heat conduction and thicknesses λ_1, H_1 and λ_2, H_2, respectively. Temperatures and heat fluxes are considered to be continuous on contact surfaces of the explosive and the walls. A zero-order chemical reaction whose rate is described by the Arrhenius equation takes place in the explosive. In the general formulation, the temperatures of the external medium and the corresponding Biot numbers have arbitrary values. The objective of the work was to investigate the critical conditions for thermal explosion.

The mathematical model of the problem in dimensionless variables is as follows:

$$d^2\Theta/d\xi^2 + \delta \exp \Theta = 0 \, , \tag{1}$$

$$d^2\Theta_1/d\xi^2 = 0 \, , \tag{2}$$

$$d^2\Theta_2/d\xi^2 = 0 \, , \tag{3}$$

$$\Theta = \Theta_1 \, , \;\; K_{\lambda 1} d\Theta/d\xi = d\Theta_1/d\xi \;\;\text{at}\;\; \xi = 0 \, ; \tag{4}$$

$$\Theta = \Theta_2 \, , \;\; K_{\lambda 2} d\Theta/d\xi = d\Theta_2/d\xi \;\;\text{at}\;\; \xi = 1 \, ; \tag{5}$$

$$\text{Bi}_2 \, (\Theta_2 - \Theta_{\text{env}2}) = - \, d\Theta_2/d\xi \;\;\text{at}\;\; \xi = K_2 \, ; \tag{6}$$

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$$\mathrm{Bi}_1 (\Theta_1 - \Theta_{\mathrm{envl}}) = d\Theta_1/d\xi \quad \text{at } \xi = -K_1 . \tag{7}$$

Here $\Theta = E(T - T_*)/RT_*^2$, $\xi = x/H$, $\Theta_1 = E(T_1 - T_*)/RT_*^2$, $\Theta_2 = E(T_2 - T_*)/RT_*^2$, $K_{\lambda 1} = \lambda/\lambda_1$, $K_{\lambda 2} = \lambda/\lambda_2$, $K_1 = H_1/H$, $K_2 = H_2/H$, $\mathrm{Bi}_2 = \alpha_2 H/\lambda_2$, $\mathrm{Bi}_1 = \alpha_1 H/\lambda_1$, $\Theta_{\mathrm{envl}} = E(T_{\mathrm{envl}} - T_*)/RT_*^2$, and $\Theta_{\mathrm{env2}} = E(T_{\mathrm{env2}} - T_*)$, and T, T_1, and T_2 are the temperatures of the reagent and the inert walls.

The unwieldy system of equations (1)-(7) does not permit an explicit expression for the critical parameter δ. However, if only critical conditions for thermal explosion are investigated, the system of equations (1)-(7) can be simplified by means of transformations using conjugation conditions (4) and (5). Upon doing this, we arrive at the following mathematical model describing the thermal explosion of a reactive layer in the case of asymmetric boundary conditions of the third kind:

$$d^2\Theta/d\xi^2 + \delta \exp \Theta = 0 , \tag{8}$$

$$\mathrm{Bi}_{0\mathrm{eff}} (\Theta - \Theta_{\mathrm{envl}}) = d\Theta/d\xi \quad \text{at } \xi = 0 , \tag{9}$$

$$\mathrm{Bi}_{1\mathrm{eff}} (\Theta - \Theta_{\mathrm{env2}}) = - d\Theta/d\xi \quad \text{at } \xi = 1 . \tag{10}$$

Here $\mathrm{Bi}_{0\mathrm{eff}} = \mathrm{Bi}_1/K_{\lambda 1}(1 + K_1\mathrm{Bi}_1)$ and $\mathrm{Bi}_{1\mathrm{eff}} = \mathrm{Bi}_2/K_{\lambda 2}(1 + K_2\mathrm{Bi}_2)$ are effective heat exchange coefficients. The effect of the inert walls on the processes of thermal explosion manifests itself via these coefficients.

The simplified system of equations (8)-(10) also does not permit obtaining the sought dependence for δ. Therefore, we made an attempt to solve the system of equations (8)-(10) by an inverse method that is reduced to setting the temperature field in the form of known temperatures on outer surfaces of the plates. Let the dimensional values of the given temperatures be T_0 and T_1, and $T_0 > T_1$. We take the higher temperature T_0 as a scale. As a result, we obtain the following boundary conditions:

$$\xi = 0 : \ \Theta = 0 ; \ \ \xi = 1 : \ \Theta = \Theta_1 . \tag{11}$$

According to the inverse method, the system of equations (8) and (11) is solved first. Its solution is given in [3], where the critical parameter of thermal explosion corresponding to the given value of Θ_1 is determined from the dependence

$$\delta_* = 2 \left(\mathrm{arch}\, a_*^{0.5} + \mathrm{arch}\, (a_* \exp(-\Theta_1))^{0.5}\right)^2 / a_* . \tag{12}$$

The critical value a_* is determined from the condition of the maximum right-hand side of Eq. (12). The temperature gradients entering boundary conditions (9) and (10) are determined from the equation for the temperature field [3]: $\exp \Theta = a/\cosh^2(m\xi - b)$. Upon substituting the values of the gradients found into (9) and (10), we obtain

$$- \mathrm{Bi}_{0\mathrm{eff}}\, \Theta_{\mathrm{envl}} = 2 \tanh (b_*)\, m_* , \tag{13}$$

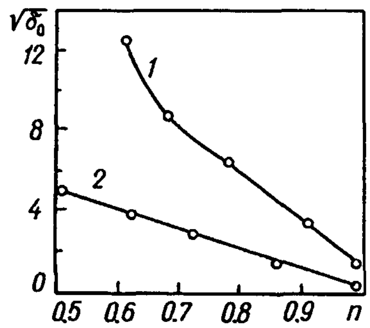
$$\mathrm{Bi}_{1\mathrm{eff}} (\Theta_1 - \Theta_{\mathrm{env2}}) = 2 \tanh (m_* - b_*)\, m_* , \tag{14}$$

where

$$b = \ln p ; \ \ p = a_*^{0.5} + (a_* - 1)^{0.5} ; \ \ m_* = \ln (pq) ;$$

$$q = (a_* \exp(-\Theta_1))^{0.5} + (a_* \exp(-\Theta_1) - 1)^{0.5} . \tag{15}$$

Upon solving Eq. (13) with respect to T_0, we obtain



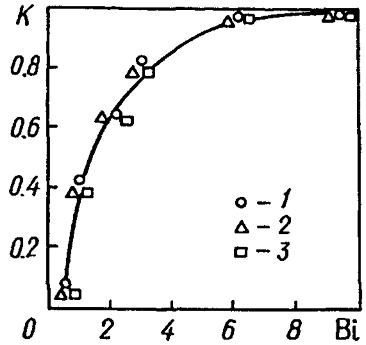


Fig. 1. Critical conditions for thermal explosion obtained from the general solution of (8)-(10): $Bi_{0eff} = 10$ and $Bi_{1eff} = 15$ (1), and $Bi_{0eff} = 1$ and $Bi_{1eff} = 5$ (2).

Fig. 2. Dependence of $K = Fk/\delta_0$ on the equivalent Biot number for $Bi_0 = Bi_1 = \infty$, $T_{env1} = T_{env2} = T_{env}$, and $H_1 = H_2 = H$ for three particular cases: $\lambda_1 = \lambda_2$, $K_{\lambda 1} = K_{\lambda 2}$, and $Bi_{0eff} = Bi_{1eff} = 1/K_{\lambda 1}$ (1), $\lambda_1 = \infty$, $K_{\lambda 1} = 0$, $K_{\lambda 2} = \lambda/\lambda_2$, $Bi_{0eff} = \infty$, and $Bi_{1eff} = 1/K_{\lambda 2}$ (2), and $\lambda_1 = 0$, $K_{\lambda 1} = 0$, $K_{\lambda 2} = \lambda/\lambda_2$, $Bi_{0eff} = \infty$, and $Bi_{1eff} = 1/K_{\lambda 2}$ (3). Fk and δ_0 are critical parameters taken from [2] and calculated by (18), respectively.

$$T_0 = zT_{env1}, \quad z = (1 - (1 - x)^{0.5})\, 2/x, \qquad (16)$$
$$x = 8 \tanh(b_*)\, m_*/Bi_{0eff}U, \quad U = E/RT_{env1}.$$

The solution of Eq. (14) allows finding the parameter

$$n_{calc} = (1 - (2 \tanh(m_* - b_*)\, m_*/Bi_{1eff} - \Theta_1)\, z/U)\, z, \qquad (17)$$

which, being compared with $n = T_{env2}/T_{env1}$, makes it possible to monitor the correctness of the choice of the value of Θ_1. The condition required is satisfied when $n_{calc} \simeq n$. It is assumed that $T_{env1} \geq T_{env2}$. If the value of n_{calc} does not coincide with the original one defined by the formulation of the problem, the iteration process is repeated.

As a result, a safe technological mode is provided when $Qk_0 \exp(-E/RT_1)EH^2/\lambda RT_1^2 < \delta_*$. The left-hand side of this inequality is the actual value of the parameter δ, which is calculated in the literature for the temperature of the environment. Upon passing from T_1 to T_{env1} using (12), we obtain the following dependence:

$$Qk_0 \exp(-E/RT_{env1})\, EH^2/\lambda RT_{env1}^2 < \delta_0, \qquad (18)$$
$$\delta_0 = \delta_* z^2 \exp(-U(1 - 1/z)).$$

Let us consider certain results of numerical calculations obtained using Eq. (18) for the general case and particular cases. Results of calculations for the general case when Bi_1 # Bi_2 and T_{env1} # T_{env2} are presented in Fig. 1 in the form $\delta_0 = f(n)$. It is evident that the value of the critical parameter increases with decreasing n and increasing Bi, since under these conditions the cooling effect is enhanced. The results obtained correspond to published data. From the general solution, one can obtain particular solutions considered earlier in [2].

1. Let $Bi_1 = Bi_2 = \infty$ and $T_{env1} = T_{env2} = T_{env}$ on the outer surfaces of the inert walls. In addition, $\lambda_1 = \lambda_2$ and $H_1 = H_2 = H$. As a result, we have $K_1 = K_2 = 1$ and $Bi_{0eff} = Bi_{1eff} = 1/K_{\lambda 1}$. The problem of the thermal explosion of the three-layer system is reduced to that for a single-layer system under symmetric boundary conditions of the third kind. Results of calculations by Eq. (18) are presented in Fig. 2 along with data from [2]. The data are

compared by the value of $K = \delta_0/\text{Fk}$, where Fk is the critical parameter of thermal explosion of the problem considered, according to [2].

2. One of the inert walls has infinite thermal conductivity, and the other has an arbitrary value of this parameter. We assume that $\text{Bi}_1 = Bi_2 = \infty$, $T_{\text{env1}} = T_{\text{env2}} = T_{\text{env}}$, $H_1 = H_2 = H$, and $\lambda_1 = \infty$. Under these conditions, $\text{Bi}_{0\text{eff}} = \infty$ and $\text{Bi}_{1\text{eff}} = 1/K_{\lambda 2}$. Thus, we have a problem of the thermal explosion of a single-layer reagent one of whose surfaces is maintained at a constant temperature T_{env}, and convective heat transfer takes place on the other surface. Results of calculations are compared in Fig. 2.

3. One of the walls is a thermal insulator. For definiteness, let $\lambda_1 = 0$. In addition, it is assumed that $\text{Bi}_1 = \text{Bi}_2 = \infty$ and $T_{\text{env1}} = T_{\text{env2}} = T_{\text{env}}$. In this case we have $\text{Bi}_{0\text{eff}} = 0$ and $\text{Bi}_{1\text{eff}} = 1/K_{\lambda 2}$. We obtain the problem of the thermal explosion of a single-layer reagent with the temperature gradient being equal to zero on one of the surfaces and convective heat transfer taking place on the other surface. In this case $H_1 = H_2 = H$. Results of calculations are compared in Fig. 2.

An analysis of the results of the calculations shows that upon solving one and the same problem by the two different methods, the values of the critical parameters differ for $\text{Bi}_{\text{eff}} < 7$ and coincide for $\text{Bi}_{\text{eff}} > 7$. The difference between the results of the calculations can be explained by the circumstance that different scaling temperatures are used in the calculations: the temperature of the environment T_{env} in [2] and the temperature on the reagent surface T_0 in the present work. The relationship between these temperatures depends on the Bi_{eff} number. For small Bi_{eff}, T_0 and T_{env} have different values ($T_0 > T_{\text{env}}$), and $T_0 \to T_{\text{env}}$ with increasing Bi_{eff}. Therefore, when $\text{Bi}_{\text{eff}} > 7$, the results of evaluation of the critical parameter are virtually coincident, since in the two works scaling temperatures with insignificantly different values are used.

Thus, we have shown that, for relatively small values of Bi, the value of the critical parameter depends strongly on the choice of the scaling temperature in the vicinity of which the Frank-Kamenetskii exponential transformation is carried out. In the monograph [3] devoted to thermal explosion under asymmetric boundary conditions of the first kind, the choice of the highest temperature on the surface as the scaling temperature is recommended. In view of this recommendation, the use of T_1 as the characteristic temperature is more substantiated, since $T_0 > T_{\text{env}}$ for small Bi. The problem of the thermal explosion of a plate under symmetric boundary conditions investigated for variable T_* has also shown that growth of the scaling temperature leads to underestimation of the value of the critical parameter δ_0. It should be noted that a change in the parameter U from 30 to 50 for Bi > 1 has virtually no effect on the value of δ_0.

Evaluation of the critical value a_* from Eq. (12), which satisfies the condition $d\delta/da = 0$, is connected with certain computational difficulties in engineering practice. The following approximate formulas are proposed for reducing the amount of engineering calculations:

$$-\Theta_1 = 340.11/\exp(a) + 80.224 \ln a - 109.95/a - 22.738a \quad (0 \le a \le 2.152),$$

$$-\Theta_1 = 1/(19.255a - 17.586/a - 32.339 \ln a - 1.6183a^2) \quad (1.043 \le a \le 2.152),$$

$$-\Theta_1 = 1/(-6.9144 \exp(a) + 39.664 \ln a + 18.827/a) \quad (1.0188 \le a \le 1.043),$$

$$-\Theta_1 = 1/(235.72/\exp(a) + 1.0754a^2 - 87.772/a) \quad (1.0105 \le a \le 1.0188).$$

When Θ_1 is calculated by the approximate relationships, the relative error does not exceed 1% for a lying within the range of 1.0105 to 3.2760. In this case the value of $-\Theta_1$ lies in the range of 0–20.

Let us consider an algorithm for evaluation of the critical conditions for thermal explosion in engineering calculations. Let the thermophysical parameters of the reagent and the inert walls, the kinetic parameters of the reagent, and the boundary conditions on the outer surfaces of the walls be known. Given the values of $\text{Bi}_{0\text{eff}}$, $\text{Bi}_{1\text{eff}}$, and $n = T_{\text{env2}}/T_{\text{env1}}$, from (17) values of a and Θ_1 that satisfy the condition $n_{\text{calc}} \cong n$ are found based on the approximating functions by the trial-and-error method. Then the critical parameter δ_0 is calculated by (18), and the values of b, m, and z entering the formulas for the calculations are evaluated by Eqs. (14), (15), and (16). The relative error of evaluation of δ_0 by the engineering method does not exceed 1%.

NOTATION

Θ, Θ_1, and Θ_2, dimensionless temperatures of the chemical substance and the inert walls, respectively; $\delta_0 = Qk_0 \exp(-E/RT_*)EH^2/\lambda RT_*^2$, Frank-Kamenetskii parameter; x and ξ, dimensional and dimensionless coordinates; Q, thermal effect of the reaction; k_0, preexponential factor; E, activation energy; R, gas constant; T_*, scaling temperature; T_0 and T_1, temperatures of the hot and cold reagent surfaces; α_2 and α_1, heat transfer coefficients; T_{env1} and T_{env2}, temperatures of the environment; Bi_2 and Bi_1, Biot numbers; Θ_{env1} and Θ_{env2}, dimensionless temperatures of the environment.

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