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CONJUGATE PROBLEM OF A THERMAL EXPLOSION WITH BOUNDARY CONDITIONS OF THE SECOND KIND

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The problem of the thermal explosion of a reagent in the form of a plane layer that is in contact with an inert plate is solved analytically with boundary conditions of the second kind. Critical conditions for the thermal explosion, depending on the heat-flux density and the kinetic and thermophysical parameters of the plate, are investigated. An engineering method for determination of the critical conditions for the thermal explosion is proposed.

Practical demands of industry constantly pose problems related to the development of high-energy explosives that possess increased sensitivity to thermal and mechanical effects. Adoption of these explosives in production requires theoretical and experimental study of them to provide technological safety. The theory of thermal explosion occupies an important place in such studies. Most studies devoted to thermal explosion are generalized in [1]. Thermal explosions occur mostly in explosive-processing apparatuses. Therefore, problems of the thermal explosion of explosives under production conditions must be modeled with account for the effect of the inert walls of the apparatus or its elements on thermal processes. The thermal explosion of a reagent confined between two inert walls has been investigated numerically and analytically in [2, 3] with boundary conditions of the first and third kind. We make an attempt to solve the conjugate problem of a thermal explosion with boundary conditions of the second kind on the exterior surface of the reagent. The formulation of the problem is as follows. A condensed explosive in the form of an infinite plate with a thickness h and a thermal conductivity λ is in close contact with an inert plate whose thickness and thermal conductivity are h_w and λ_w, respectively. The open surface of the explosive is affected by a constant heat flux. The other open surface of the inert plate is kept at constant temperature. The temperature and the heat flux on the surface of contact between the explosive and the inert wall are continuous. There is an internal nonlinear chemical source of heat in the explosive. A zero-order chemical reaction whose rate is described by the Arrhenius equation is considered. The objective of the work is to investigate the critical conditions for a thermal explosion in the formulation considered.

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

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

$$d^2 v/d\xi^2 = 0 \; ; \tag{2}$$

$$\sigma = -\, d\theta/d\xi \quad \text{at} \quad \xi = -1 \; ; \tag{3}$$

$$\theta = v \, , \quad d\theta/d\xi = K_\lambda \, dv/d\xi \quad \text{at} \quad \xi = 0 \; ; \tag{4}$$

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TABLE 1. Relative Decrease in the Critical Parameter

Wall material	λ_w, W/(m·K)	K_λ	K_h	ε, %
Steel	45.28	361	1.0	0.4
Textolite	0.34	2.71	1.0	34
Rubber	0.16	1.30	1.0	50

$$v = \theta_0 \quad \text{at} \quad \xi = K_h \,. \tag{5}$$

Here $\theta = E(T - T_*)/(RT_*^2)$, $\xi = x/h$, $v = E(u - T_*)/(RT_*^2)$, $\sigma = qEh/(\lambda RT_*^2)$, $K_\lambda = \lambda_w/\lambda$, $K_h = h_w/h$, $\delta = Qk_0 \exp(-E/RT_*)Eh^2/(\lambda RT_*^2)$, and $\theta_0 = E(T_0 - T_*)/(RT_*^2)$.

As the scaling temperature T_* we take the temperature on the surface ($\xi = -1$) obtained from solution of the system of equations (1)–(5) in the inert formulation neglecting the heat of chemical reactions:

$$T_* = T_0\,(1 + \mathrm{Ki}\,(1 + K_h/K_\lambda))\,, \tag{6}$$

where $\mathrm{Ki} = qh/(\lambda T_0)$.

In (1), the transformation of the exponent in the Arrhenius equation according to Frank-Kamenetskii [4] is used.

The solution of Eq. (1) that satisfies the boundary conditions makes it possible to obtain a stationary distribution of temperature only for $\delta < \delta_{cr}$. The thermal explosion in the formulation of Frank-Kamenetskii [4] occurs when $\delta > \delta_{cr}$. There is no stationary solution to the problem posed under these conditions. Thus, finding the critical conditions of a thermal explosion is reduced to determination of δ_{cr} from the solution of the system of equations (1)–(6).

We solve system (1)–(6) in order to determine the critical conditions for a thermal explosion. The relatively complex system of equations is simplified if we solve Eq. (2) with boundary conditions (4)-(5) and, having determined $dv/d\xi = (\theta - \theta_0)/K_h$, substitute it into (4). Then, instead of the conjugate problem, we obtain the following equivalent problem of a thermal explosion for the reagent:

$$d^2\theta/d\xi^2 + \delta \exp\theta = 0\,, \tag{7}$$

$$\sigma = -\,d\theta/d\xi \quad \text{at} \quad \xi = 0\,, \tag{8}$$

$$K\,(\theta - \theta_0) = -\,d\theta/d\xi \quad \text{at} \quad \xi = 1\,, \tag{9}$$

where $K = K_\lambda/K_h$. The conjugate problem with boundary conditions of the second and first kind changes to the problem of a thermal explosion with boundary conditions of the second and third kind, where K is an analog of the Biot criterion. The sought values of the critical parameter δ_{cr} are found from the solution of (7)–(9).

The solution of Eq. (7) is written in the form [4]

$$\exp\theta = a/\cosh^2(\mu\xi + b)\,, \tag{10}$$

where a and b are the integration constants and $\mu = (a\delta/2)^{0.5}$. On the basis of (10) the boundary conditions (8) and (9) acquire the form

$$\sigma = 2\tanh(b)\,\mu\,, \tag{11}$$

$$K\,(\ln a - 2\ln\cosh(b + \mu) - \theta_0) = 2\tanh(b + \mu)\,\mu\,. \tag{12}$$

From (11) we obtain that b = arctanh ($\sigma/(2\mu)$).

Having solved (12) for a, we obtain

$$a = \exp(\theta_0 + 2 \ln\cosh(b + \mu) + 2 \tanh(b + \mu)\, \mu/K) . \tag{13}$$

Using the relation $\mu^2 = a\delta/2$ mentioned earlier [4], from Eq. (13) we obtain

$$\delta = 2\mu^2/\exp(\theta_0 + 2 \ln\cosh(b + \mu) + 2 \tanh(b + \mu)\, \mu/K) . \tag{14}$$

The critical condition for a thermal explosion is determined by the maximum of the right-hand side of (14) as a function of μ. An analysis showed that the condition for a maximum holds for $d\delta/d\mu = 0$. Therefore, having differentiated (14) with respect to μ and having equated the derivative to zero, we obtain the following transcendental equation for determining μ_*, for which δ takes the critical value:

$$(\mu_* - z/(1 - z^2)) \tanh(b + \mu_*) + \mu_* [(\mu_* - z/(1 - z^2))/\cosh^2(b + \mu_*) + \tanh(b + \mu_*)]/K = 1 , \tag{15}$$

where $z = \sigma/(2\mu_*)$. Having calculated the value of μ_* from (15) by the iteration method, we can find the critical Frank-Kamenetskii parameter from the following equation:

$$\delta_{cr} = 2\mu_*^2/\exp(2 \tanh(b_* + \mu_*)\, \mu_*/K + 2 \ln\cosh(b_* + \mu_*) + \theta_0) , \tag{16}$$

where b_* = arctanh ($\sigma/(2\mu_*)$).

When $\lambda_w \to \infty$ and $K \to \infty$, the conjugate problem considered changes to the problem of the thermal explosion of a flat body without a substrate. In this case, the approximating function

$$(\delta_{cr})_\infty = (0.1344\sigma^2 + 0.4135\sigma + 0.7804)^{0.5} . \tag{17}$$

is suggested for engineering calculations.

In calculating δ_{cr} by (17), the relative error within the range of variation of σ from 0 to 20 does not exceed 1%. A study of the effect of inert walls on the critical Frank-Kamenetskii parameter is of interest. For this purpose, the critical parameters for an explosive with and without a substrate are compared. The approximating function that allows for the effect of inert walls on the critical parameter has the form

$$\delta_{cr} = (\delta_{cr})_\infty\, \varphi(K)\, (0.57 + K)/K , \tag{18}$$

where $\varphi(K) = K((K^2 + 4)^{0.5} - K) \exp(((K^2 + 4)^{0.5} - K - 2)/K)/2$. This formula, suggested in [5], where K = Bi, takes into account the dependence of the critical parameter δ on the Biot criterion in problems with boundary conditions of the third kind. Barzykin et al. [5] noted that the indicated formula, which is accurate for the thermal explosion of an infinite cylinder, also holds with good accuracy (1–2%) for other bodies. In this work, it can be considered as a computational finding for the approximating function. The relative error of (18) within the range of variation of K from 2 to ∞ does not exceed 8%.

In concluding, we determine the effect of an inert wall on the decrease in the critical parameter for certain particular cases quantitatively. Calculation results are given in Table 1. The relative decrease in the critical parameter (%) is calculated from the dependence $\varepsilon = ((\delta_{cr})_\infty - \delta_{cr})\cdot 100/(\delta_{cr})_\infty$. The calculations are done by the approximating functions (17) and (18) for λ_{expl} = 0.1254 W/(m·K).

It is seen from Table 1 that, under the conditions considered, an inert steel wall virtually does not affect the critical parameter. However, the effect of inert walls made of heat-insulating materials on the critical parameter is substantial. Values of ε within the wide range of variation of K from 1 to 50 that are determined from Eq. (16) and the approximating functions (17) and (18) are presented in Fig. 1. It is seen from

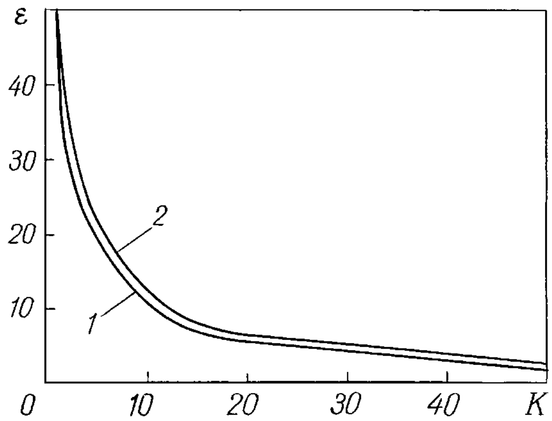

Fig. 1. Effect of an inert wall on the change in the critical parameter: 1) by Eq. (16); 2) by the approximating functions (17) and (18). ε, %.

the figure that ε calculated by the approximating functions are in satisfactory agreement with results obtained from Eq. (16). In this case, the relative error does not exceed 8%. If for the sake of analysis of the figure we take $K_h = 1$, then $K = \lambda_w/\lambda_{expl}$. For small λ_w, the inert wall plays the role of a heat-insulator, which facilitates enhancement of thermal processes in the reagent, and, as a consequence, the thermal explosion occurs for smaller δ_{cr} compared to the case of the absence of an inert wall. Thus, for $\lambda_w = \lambda_{expl}$ the decrease in ε is about 50%. Under these conditions, there is virtually no effect of the steel wall on the critical parameter, since $K > 50$ and, as is seen from the figure, for these values $\varepsilon \to 0$.

Thus, the problem of the thermal explosion of an explosive in the form of a plate that is in close contact with an inert material is solved with mixed boundary conditions for the second and first kind. The critical conditions for the thermal explosion are studied and a transcendental equation that determines the critical Frank-Kamenetskii parameter is obtained. Engineering formulas are suggested for calculating the critical parameter.

NOTATION

θ and T, dimensionless and dimensional temperatures of the explosive; T_*, scaling temperature; ξ, dimensionless coordinate; h, thickness of the explosive plate; h_w, thickness of the inert wall; u and v, dimensional and dimensionless temperatures of the inert wall; δ, Frank-Kamenetskii parameter; δ_{cr}, critical Frank-Kamenetskii parameter; E, activation energy; R, gas constant; Q, thermal effect of the reaction; k_0, preexponential factor; λ and λ_w, coefficients of thermal conductivity of the explosive and the wall; q and σ, dimensional and dimensionless heat-flux densities; θ_0 and T_0, dimensionless and dimensional temperatures of the environment; Ki and Bi, Kirpichev and Biot criteria; K_λ, dimensionless coefficient of thermal conductivity; K_h, dimensionless thickness; $(\delta_{cr})_\infty$, critical parameter for $K \to \infty$. Subscripts: *, characteristic quantity; w, wall; 0, initial state of parameters; cr, critical.

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