IGNITION OF A CONDENSED EXPLOSIVE BY A HOT

OBJECT OF FINITE DIMENSIONS

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Study of ignition due to contact of an explosive with a hot inert object is of interest primarily in connection with the problem of the Sensitivity of explosives to mechanical effects. The most common concept in the theory of sensitivity is that of the thermal nature of the initiation of an explosion. It is assumed [1] that various mechanical agents cause (by virtue of the dissipation of their energy) local regions of heating, from which the explosion develops. Without going into the mechanism for the appearance of these regions, we can formally divide them into two groups: reacting and inert. In the first case there is a local heating of the explosive which leads to a local thermal explosion [2]. In the case of inert regions, which arise, e.g., due to the adiabatic compression of gaseous inclusions accompanying friction between the explosive and solid particles, etc., the process develops near the interface between the hot and inert material and the cold explosive, i.e., is an ignition process.

The problem of the ignition of explosives by a hot object is of interest in connection with studies of ignition by a disperse flow [3], carried out to evaluate the role played by the penetration of the particle into the surface of the combustible material.

Numerical methods were used in $[4]$ to study one limiting case $-$ that of ignition by an inert plate having a poor thermal conductivity. Another limiting case, in which the igniting object has a good thermal conductivity, was studied in [5]. An approximate calculation of the basic characteristics of the process is reported in [4, 6].

We have now used a computer to solve the problem of the ignition of an explosive by a hot object of a symmetric shape (a plate, cylinder, or sphere) over broad ranges of the parameters involved.

The problem is formulated in the standard manner for ignition theory. In an unbounded medium capable of exothermic conversion in a condensed phase, there is a hot inert object having a characteristic dimension of 2r. The initial temperature of the explosive is T_e , and that of the hot object is T_0 . Depletion of the explosive is neglected; i.e., degenerate regimes [7] are not considered. The thermophysical properties (the thermal conductivity, heat capacity, and density) of the objects in contact and the properties of the chemical reaction (the activation energy, the heat of combustion, and the preexponential factor) in the medium are assamed constant over the course of the process.

The mathematical problem reduces to one of solving the following system of differential equations. written in dimensionless form: the equation describing heat propagation in the reacting substance,

$$
\frac{\partial \theta}{\partial \tau} = \frac{1}{\delta^2} \left[\frac{\partial^2 \theta}{\partial \xi^2} + \frac{n}{\xi} \frac{\partial \theta}{\partial \xi} \right] + \exp \frac{\theta}{1 + \beta \theta}, \quad 1 < \xi < \infty;
$$
\n(1)

the corresponding equation in the igniting medium,

$$
\frac{\partial \theta_1}{\partial \tau} = \frac{k_\lambda b}{\delta^2} \left[\frac{\partial^2 \theta_1}{\partial \xi^2} + \frac{n}{\xi} \frac{\partial \theta_1}{\partial \xi} \right], \quad 0 < \xi < 1; \tag{2}
$$

and the initial and boundary conditions,

$$
\tau = 0, \quad \theta_1 = 0, \quad \theta = -\theta_{\rm s}, \tag{3}
$$

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$$
\xi = 0, \quad \frac{\partial \theta}{\partial \xi} = 0, \quad \xi \to \infty, \quad \theta = -\theta_{\xi}, \tag{4}
$$

$$
\xi = 1, \ \theta_1 = \theta, \quad k_{\lambda} \frac{\partial \theta_1}{\partial \xi} = \frac{\partial \theta}{\partial \xi}.
$$

For the case $k\lambda \rightarrow \infty$ we replace Eq. (2) and boundary conditions (5) by

$$
\xi = 1, \quad \frac{\partial \theta}{\partial \tau} = \frac{(n+1)}{\delta^2} b \frac{\partial \theta}{\partial \xi}, \quad \theta_1 = \theta.
$$
 (6)

Here

$$
\theta = \frac{E}{RT_0^2} (T - T_0); \quad \xi = \frac{x}{r}; \quad \beta = \frac{RT_0}{E};
$$

$$
\tau = t \frac{Qk_0}{c\rho} \frac{E}{RT_0^2} \exp(-E/RT_0);
$$

$$
\delta = r \left[\frac{Qk_0}{\lambda} \frac{E}{RT_0^2} \exp(-E/RT_0) \right]^{1.2};
$$

$$
k_{\lambda} = \frac{\lambda_1}{\lambda}; \quad b = \frac{c\rho}{c_1 \rho_1}; \quad \theta_e = \frac{E}{RT_0^2} (T_0 - T_e);
$$

x is the coordinate; t is the time; T is the temperature; Q is the heat of combustion; E is the activation energy; λ , c, and ρ are the thermal conductivity, heat capacity, and density, respectively; n is the shape index; and the subscript $"1"$ corresponds to the igniting object.

Solving the initial system of equations numerically on a computer, we obtained the nonsteady-state temperature fields $\theta(\xi, \tau, \theta_{\theta}, k_2, b, \beta, \delta, n)$, from which we determined the basic characteristics of the ignition. The parameter ranges taken into consideration are $\theta_e = 7.5-25$; $\delta = \delta_{cr} - \infty$; $0.01 < \beta < 0.9/\theta_e$; $k_A =$ 0.1- ∞ ; b=0.05-100; and n=0, 1, 2.

Figure 1 shows the time dependence of the temperature $\theta_{\rm S}$ at the interface between the inert object and the reacting material for various values of the parameter δ . This temperature instantaneously assumes a certain value θ_{S} , and, at sufficiently large values of δ , remains constant throughout the ignition. As δ decreases, the value of θ_S decreases as time elapses (the rate at which the temperature drops is governed by the heat reserve in the heating region and by the thermophysical and kinetic properties of the objects in contact); thereafter, it increases in an explosive manner. Finally, for dimensions $\delta < \delta_{cr}$ of the heating region, ignition does not occur. Since an adiabatic regime is possible in our formulation of the problem, we understand by "ignition" the process whose development time is much shorter than the adiabatic induction period at the initial temperature θ_{Θ} .

Since the transition from the ignition regime to that of adiabatic combustion occurs continuously, there is some difficulty in choosing $\delta_{\rm cr}$. Analysis of the $\tau_i(\delta)$ dependences shows that we can determine δ_{cr} by using the condition $\frac{\Delta \tau_i}{\Delta \delta} \gg 1$ as a criterion: At values near δ_{cr} (Fig. 2b), a slight change in the dimension of the heating region corresponds to a large change in the ignition delay time.

It has been shown [7, 8] that for the case in which a surface is heated by conduction the ignition characteristics can be described very accurately by the equations obtained for the case of ignition at a constant surface temperature; the surface temperature should be identified as the temperature of the interface, known from the theory of heat conduction:

$$
T_{s_1} = (T_0 - T_{\rm e}) \frac{k_e}{1 + k_{\rm e}} + T_{\rm e} ,
$$

where $k_F = (\lambda_1 c_f \rho_1 / \lambda c \rho)^{1/2}$ is the ratio of thermal activities.

From Fig. 2 we see that this conclusion holds for our case, beginning at some δ/δ_{cr} . As δ/δ_{cr} increases, the time τ_i tends toward [8]

$$
\tau_{\mathbf{i}}^{\mathbf{I}} = 0.2\theta_{s_1}(\theta_{s_1} + 8),\tag{7}
$$

where

$$
\theta_{s_1} = \frac{E}{RT_{s_1^*}^*} (T_{s_1} - T_{e}).
$$

Fig. 1. Dependence of θ_S on τ for various values of δ , with $\theta_n = -10$, $\beta = 0.01$, $k_\lambda = 20$, $b = 0.06$, and $n = 2$. 1) $\delta = 1000; 2$ $\delta = 30; 3$ $\delta = 21; 4$ $\delta = 20; 5$ $\delta = 19; 6$ δ = 21, corresponding to heat exchange with the inert medium.

Fig. 2. a) Dependence of τ_i/τ_i^1 on δ/δ_{cr} ; b) dependence of τ_1 on δ for a cylinder with $\theta_e = -10$, $\beta = 0.01$, $k_{\lambda} \rightarrow \infty$, and b=0.1. 1) Sphere; 2) plane.

Fig. 3. Dependence of δ_{cr}^* and $\delta_{\text{cr}}/\delta_{\text{cr}}^*$ on b for $\theta_{\text{e}} = -10$, $\beta =$ 0.01, and n=0. 1) $k_{\lambda} \rightarrow \infty$; 2) k_{λ} = 100; 3) k_{λ} = 10; 4) k_{λ} = 1.

We note that we have τ_i/τ_i^{\to} 1 within ~5% for $\delta/\delta_{\text{cr}} > 1.8$, corresponding to a temperature of the heating region which is higher than the critical temperature by about half the temperature interval $(\sim 10^{\circ})$.

We are primarily interested in finding the critical conditions. Figure 3 shows typical dependences of $\delta/\delta_{\text{CT}}^*$ on b for various values of k_{λ} ; here δ^* corresponds to ignition of the explosive by a heating region of infinite thermal conductivity $(k_{\lambda} \rightarrow \infty)$. Analysis of these dependences reveals the existence of three limiting regimes:

1) $b \rightarrow 0$, $k\lambda > 0$ (infinite heat capacity of the heating region). The ignition occurs for any size of the heating region $(\delta_{cr} \rightarrow 0)$.

2) b $\rightarrow \infty$, k_{λ} > 0 (vanishingly small heat capacity of the heating region). Here we have $\delta_{cr} \rightarrow \infty$, and the combustion occurs in the adiabatic regime.

3) $k_{\lambda} \rightarrow 0$, b>0. The heat flux is $k_{\lambda} \frac{\partial \theta}{\partial \xi} \Big|_{\xi=1}$, and the combustion occurs in the adiabatic regime.

It should be noted that the case $k_{\lambda} \rightarrow \infty$ corresponds to a quite large range $k_{\lambda} > 100$ over which the critical dimension of the heating region is essentially independent of k_{λ} and over which we have $\delta_{cr} = \delta_{cr}^*$ $(Fig. 3)$.

The dependences of δ_{cr} and δ_{cr}^* on the parameters θ_{θ} , β , k_{λ} , b, and n can be described approximately

by

$$
\delta_{\text{cr}}^{\bullet} = 0.4 \sqrt{b^2 + 0.25n(n+1)(b+0.1b^2)} \left[\theta_{\text{e}} + 2.25(n-1) \right]^2 \left[1 + 0.5\beta \theta \right],\tag{8}
$$

$$
\delta_{\rm cr} = \delta_{\rm cr}^* \left[1 + \frac{(\theta_{\rm c} - 3)^2 b (n+1)}{30 k_{\rm a}^{2/3} (1 + 3b^{2/3})} \right]. \tag{9}
$$

These equations hold within 10% over the following parameter ranges: $\theta_e = 7.5-25$; $\beta = 0.01-0.9/\theta_e$; n= 0, 1, 2; $k_{\lambda} = 1-\infty$; b=0.05-10. For $k_{\lambda} = 0.1-1$ and b=10-100, Eqs. (8) and (9) give δ_{CT} within ~20%.

Some results of the numerical integration and some values of δ_{cr} calculated from Eqs. (8) and (9) are compared in Table 1 with results† obtained by the approximate methods of $[4, 6]$ and through a numerical calculation for $k_{\lambda} \rightarrow \infty$ [5]. We see that the values of δ_{cr} calculated by the approximate methods of [4, 6] agree satisfactorily with the results of the computer calculations of the present study and of [5]. We note that for the cases of a cylinder $(n=1)$ and a sphere $(n=2)$ these approximate methods require a numerical integration.

These results are of definite interest in connection with the problem of the sensitivity of explosives to mechanical effects.

The mechanism for the detonation of nitroglycerine by solid particles was discussed in [1]. We can use Eqs. (8) and (9) to calculate the critical temperature of the heating region as a function of its dimension. The initial kinetic and thermophysical properties for nitroglycerine are, according to $[1]$, $E = 48,000$ cal/mole, $Qk_0 = 5 \cdot 10^{22}$ cal/sec \cdot cm³, c = 0.3 cal/g \cdot deg, $\rho = 1.4$ g/cm³, and $\lambda = 4 \cdot 10^{-4}$ cal/cm \cdot sec \cdot deg. Those for carborundum (the igniting object) are $c = 0.18$ cal/g, $de{deg}$, $p = 2.3$ g/cm³, and $\lambda = 2 \cdot 10^{-3}$ cal/cm. sec - deg. Then we find the following critical temperatures for the specified dimensions of the heating region:

$$
d, \mu \qquad 100 \qquad 50 \qquad 10 \qquad 0.5
$$

$$
\widetilde{T}_{\text{C}r} \qquad {}^{\circ}C \quad 391 \quad 448 \quad 519 \quad 639
$$

The calculated results are in good qualitative agreement with the experimental data of [1], where it was shown that large carborundum particles $\sim 100 \mu$ in size) are more efficient in forming heating regions (explosions occur in 100% of the cases) than small particles $(0.5-10 \,\mu)$; the temperatures of the heating regions were measured and found to be $\sim 500^{\circ}$ C.

Analogous calculations were carried out for the case in which there is a gas bubble in nitroglycerine. In this case the detonation of the explosive can be attributed to the adiabatic compression and heating of the gas upon impact. Experimental temperatures prevailing during impact compression were given for certain gases in [1]; for air, for example, the value is $T_{cr} = 800^{\circ}C$. However, the calculations showed that for the detonation of nitroglycerine by an air bubble having an initial diameter of 1 mm the critical temperatures are much higher: $T_{cr} = 1200^{\circ}$ C. These results support the hypothesis of [1] that detonation occurs during adiabatic compression of a bubble if the air inclusions contain explosives as a vapor or small drops.

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tit is difficult to compare our results with those of the numerical calculation of [4], because the range of the parameter k_{λ} was not specified there.