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LAWS OF IGNITION OF CONDENSED EXPLOSIVE SYSTEMS WITH PERFECT HEAT TRANSFER AT THE SURFACE AND ALLOWANCE FOR BURNUP

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An electronic computer has been used to obtain the ignition characteristics of nonvolatile explosive systems with allowance for burnup of the substance during the reaction. The results are presented as approximate formulas.

Calculations have been made for the ordinary simple model of a uniform exothermic reaction of the first order in the condensed phase with unsteady heat conduction without allowance for possible complicating physical and chemical processes (phase transformations in the interior and at the surface of the condensed substance, multiphase conditions, physical or kinetic, dispersal of the condensed phase by expansion of the gaseous reaction products, etc.).

Specific formulation of the problem. The condensed substance, which is capable of an exothermic reaction and semi-infinite in extent*, is brought into contact with a source whose temperature T_0 exceeds the initial temperature T_i of the substance; it is assumed that the surface temperature equals T_0 and does not change with time.

The set of equations describing the first-order reaction, with allowance for depletion of the substance, and the boundary conditions, all in dimensionless variables, take the form

$$\frac{\partial\vartheta}{\partial\tau} = \frac{\partial^2\vartheta}{\partial\xi^2} + (1-\eta)\exp\frac{\vartheta}{1+\beta\vartheta}; \tag{1}$$

$$\frac{\partial\eta}{\partial\tau} = \gamma(1-\eta)\exp\frac{\vartheta}{1+\beta\vartheta}; \tag{2}$$

$$\tau = 0, \quad \vartheta = -\vartheta_i, \quad \eta = 0; \tag{3}$$

$$\xi = 0, \quad \vartheta = 0; \tag{4}$$

$$\xi \to \infty, \quad \partial\vartheta/\partial\xi \to 0. \tag{5}$$

The dimensionless variables:

$$\eta; \quad \vartheta = \frac{E}{RT_0^2}(T - T_0);$$

$$\xi = x\left[\frac{Qk_0E}{\lambda RT_0^2}\exp\left(-\frac{E}{RT_0}\right)\right]^{1/2};$$

$$\tau = \frac{Qk_0Et}{c\rho RT_0^2}\exp\left(-\frac{E}{RT_0}\right).$$

The dimensionless parameters:

$$\vartheta_i = \frac{E}{RT_0^2}(T_0 - T_i); \quad \beta = \frac{RT_0}{E}; \quad \gamma = \frac{c\rho RT_0^2}{QE}.$$

The basic parameter in the problem is the temperature head ϑ_i of the source. As T_0 varies, the temperature head goes through a maximum (at $T_0 = 2T_i$), whose valie is $(\vartheta_i)_{\max} = E/4RT_i$. As $\vartheta_i \to 0$ the problem of ignition becomes meaningless.

It is known from the theory of thermal explosion that the parameter γ is a measure of burnup. Its value corresponds to the degree of decomposition when the substance is heated through the characteristic interval RT_0^2/E under adiabatic conditions. The role of γ in ignition processes has not as yet been investigated. Physically, it is clear that at small γ (low-temperature source) burnup is unimportant, while at large γ (high-temperature source), burnup may have a considerable influence. The parameter β does not usually play a significant role in ignition and burning processes.

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[*] It is known that in ignition the reaction zone is much smaller than the body dimensions, and therefore it is usual to describe the phenomenon in terms of a semi-infinite model.

The system (1)–(5) was solved numerically by means of an explicit difference scheme on a computer. The nonstationary fields of temperature $\vartheta(\xi, \tau, \vartheta_i, \beta, \gamma)$ and degree of decomposition $\eta(\xi, \tau, \vartheta_i, \beta, \gamma)$ were determined, and from these the basic characteristics of the ignition process were calculated. The range of variation of the parameters was as follows: $\vartheta_i = 3–30$, $\gamma = 0–0.3$; $\beta = 0–0.2$.

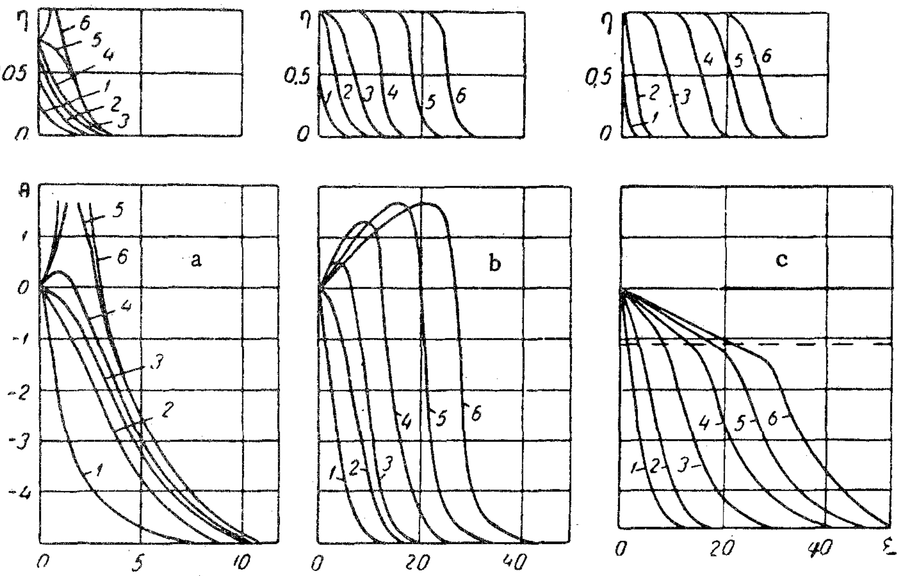

Fig. 1. Distribution of temperature and degree of deocmposition: a) $\gamma = 0.05$; $\vartheta_i = 5$; $\beta = 0.03$ (1–τ = 4.2; 2–8.4; 3–10.9; 4–12.6; 5–14.7; 6–15.1); b) $\gamma = 0.5$; $\vartheta_i = 5$; $\beta = 0.03$ (1–τ = 8.4; 2–23; 3–34; 4–50; 5–67; 6–84) c) $\gamma = 0.28$; $\vartheta_i = 4.63$; $\beta = 0.2$ (1–τ = 8.4; 2–25; 3–76; 4–143; 5–210; 6–295); $\vartheta_b = -1.06$.

The calculations showed that the development of the process depends substantially on the parameter γ. Figure 1 gives the space-time distributions of ϑ and η for various values of γ. It can be seen that at small γ (Fig. 1a), the heat buildup is self-accelerating in nature, like the development of a thermal explosion; in this case, the degree of decomposition is small. These are the normal ignition conditions. As γ increases, the explosive pattern of ignition becomes less clearly expressed, and at large γ, close to $\gamma_b = 1/\vartheta_i$ (γ_b is the value of γ at the burning temperature $T_b = T_i + Q/c\rho$), it has quite a different form (Figs. 1b and 1c). These are the degenerate ignition conditions, characterized by heavy burnup of material and a smooth transition to a process of thermal wave propagation in space. The degenerate conditions may be of two types: with self-heating ($\gamma < \gamma_b$, Fig. 1b) and without self-heating ($\gamma > \gamma_b$, Fig. 1c). In the latter case, we get forced ignition with a continuous supply of heat from the source. The transition from normal to degenerate conditions is a continuous, but fairly sharp one (Fig. 2). Analysis shows that as the value γ_{cr} separating these conditions, we may take $\gamma_{cr} = n\gamma_b$. The value of n depends weakly on the parameters and is approximately equal to 0.5.

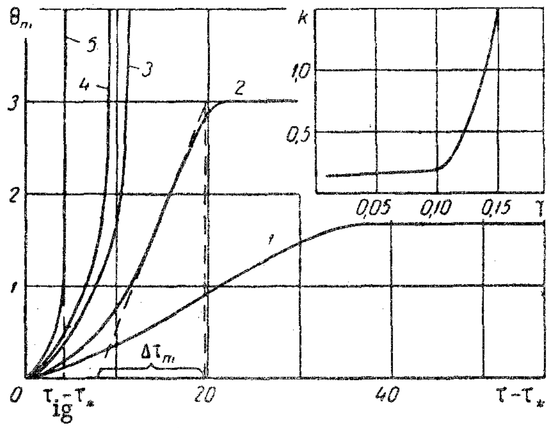

Fig. 2. Curves of maximum heat buildup with time for $\vartheta_i = 5$, $\beta = 0.03$ and various γ: 1–γ = 0.15; 2–0.25; 3–0.10; 4–0.06; 5–0.005; $k = \Delta\tau_m/\tau_*$; $\Delta\tau_m = (\gamma^{-1} - \vartheta_i)/(\partial\vartheta/\partial\tau)_{\max}$.

It should be noted that for the correct description of degenerate conditions during ignition of condensed substances, because of the intense burnup, it is necessary to allow for the removal of gaseous reaction products from the condensed phase, dispersal, etc., i.e., the use of the model in question is incorrect. In our study the ignition characteristics were calculated for normal conditions, i.e., for $0 < \gamma < \gamma_{cr}$.

The following values were determined: τ_*–"heat-up" time (time required for the heat flux at the surface to vanish); τ_d–ignition lag time; $\omega_* = \int_0^{\tau_*}\left(\frac{\partial\vartheta}{\partial\xi}\right)_{\xi=0} d\tau$ amount of heat obtained by the substance from the source during the "heatup" time; ξ_*–width of chemical reaction zone (coordinate corresponding to the value $\vartheta = -1$ at $\tau = \tau_*$). The method of determining τ_d is explained in Fig. 2. We note that for degenerate conditions, τ_d becomes indeterminate; in place of τ_d one should then introduce a value describing the time to onset of the propagation process.

To clarify the form of the dependence of τ_*, τ_{ig}, ω_* and ξ_* on the parameters ϑ_i, β, γ, a number of calculations were performed. The solution was obtained on an electronic computer to an accuracy of 6% or better. The results are presented in the form of the approximate formulas:

$$\tau_* = (\vartheta_i + 0.2\,\vartheta_i^2)(1 + \gamma\vartheta_i)(1 + \beta), \tag{6}$$

$$\omega_* = (0.7\,\vartheta_i + 0.33\,\vartheta_i^2)(1 + \gamma\vartheta_i)(1 + \beta), \tag{7}$$

$$\tau_{ig} = (1 + 1.6\,\vartheta_i + 0.2\,\vartheta_i^2)(1 + 8\,\vartheta_i\gamma^{3/2})(1 + \beta). \tag{8}$$

The formulas give an accuracy of 7% or better in the following range of variation of the parameters: $\gamma = 0$–γ_{cr}; $\vartheta_i = 3$–30; $\beta = 0$–$0.9 \cdot 1/\vartheta_i$. Without going into a detailed analysis of the laws of ignition, which could be based on the formulas obtained, we note the following:

1. Burnup is unimportant when $\gamma\vartheta_i \ll 1$ (or $\gamma \ll \gamma_b$). In this case, a zero-order reaction model may be used to investigate the phenomenon. The values of τ_{ig} for $\gamma \ll 1/\vartheta_i$, obtained from (8), agree with the theoretical data of [2] and [1] within the limits of accuracy of the calculation and approximation.

2. In some papers [3] τ_* is taken as the ignition time lag; it is then assumed that $\tau_{ig} - \tau_* \ll \tau_*$. It follows from (6) and (8) that $(\tau_{ig} - \tau_*)/\tau_*$ is indeed small for large ϑ_i and small γ. However, it grows as ϑ_i decreases and γ increases. For example, when $\vartheta_i = 5$ and $\gamma = 0.08$, the difference between τ_{ig} and τ_* is about 90% of τ_*. It is therefore clear that τ^* must not be taken as the ignition time lag in the general case.

3. The formula of Zel'dovich [3] for τ_* has the form

$$\tau_* = \vartheta_i^2/2\pi. \tag{9}$$

From an examination of the relation for $\tau_*(\vartheta_i)$ from (6) and (9) [when $\vartheta_i = 5; 10; 15; 20; 25; 30$; $\tau_* = 10; 30; 60; 100; 150; 210$, and when $\beta = \gamma = 0$ from (6), and $\tau_* = 4; 15.9; 35.8; 63.7; 99.5; 143$ from (9)], we see that the Zel'dovich formula, in the actual range of variation of ϑ_i, gives a result that is low by approximately a factor of two; the discrepancy then decreases as ϑ_i increases.

4. As the calculations show, the width of the chemical reaction zone ξ_* is practically independent of ϑ_i under normal conditions. For estimation purposes we may put $\xi_* \approx 2$.

We also made calculations for the pulse problem (the source does not act for the whole time, but only during a certain interval τ^0). It is known that in this formulation, critical ignition conditions apply. The value of τ_{cr}^0 depends on the boundary conditions, which are imposed after the source is withdrawn. If when $\tau > \tau^0$ the source temperature decreases in a jump from T_0 to T_i, then $\tau_{cr}^0 \approx \tau_{ig}$ [as an example, we give the dependence of τ_{cr}^0 and τ_{ig} on ϑ_i ($\gamma = 0.005$; $\beta = 0.03$); when $\vartheta_i = 5; 10; 15; 20$, $\tau_{cr}^0 = 13.9; 38.5; 74.5; 172.0$, and $\tau_{ig} = 15.1; 39.1; 75.4; 128.0$]; when $\tau > \tau^0$ and there is no heat transfer to the surrounding medium, $\tau_{cr}^0 = k\tau_*$, where $k < 1$. Using the calculations of [5], we obtain $k = 0.66$–0.83.

We note that in the first approximation, not allowing for diffusion and hydrodynamic effects, the above results may also be applied to the ignition of gases.

NOTATION

T—temperature; t—time; x—coordinate (distance from surface); ρ—density; c—specific heat; λ—thermal conductivity; E—activation energy; k_0—preexponent; Q—thermal effect of reaction (in unit volume); R—universal gas constant; η—degree of decomposition (ratio of amount of reacted material per unit volume at time t to initial amount of material); ϑ—temperature; ξ—space coordinate.

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