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COMBUSTION, EXPLOSION, AND SHOCK WAVES

Hot-Spot Ignition of Solid Propellants by a Hot Surface

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Abstract—The combustion of homogeneous energetic materials such as ballistic powders and explosives usually begins with the formation of a hot spot. This paper studies the conditions for an occurrence of a hot spot in case of heating by a hot surface with constant temperature. It is shown that the hot spot is formed at a certain depth under the surface, and the specific location of the hot spot depends on the geometry of the surface. Dimensionless criteria are reported for the estimation of this depth and prediction of the precise location of the hot spot. Some limit cases are studied and the function of the ignition time of a rough surface with protrusion of different heights and angles are found for several geometries of the surface.

Keywords: combustion of propellants, combustion instability, ignition hot spots, critical phenomena, combustion theory

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INTRODUCTION

The combustion of energetic materials, such as homogeneous propellants and explosives, is a multistage process that is difficult for modeling and experimental study [1, 2]. The main chemical transformations in the combustion zone occur in a very short time; and studying processes near the phase boundary, where the chemical reactions are most intense in a narrow near-surface layer, is particularly difficult. At the same time, the experimental data accumulated to date [3, 4] indicate that many significant features of the combustion of condensed substances are due to the phenomena in the so-called hot spots: small areas of the substance in comparison with the spatial scale of the sample, where the chemical reaction is currently most intense.

Ignition as the initial stage of combustion begins with the formation of a small hot spot where the local maximum of heat release occurs due to the inhomogeneity of external heating and the substance itself, as well as the presence of cracks and surface roughness and other factors [5]. The study of ignition in hot spots is extremely important for the safety of handling high-energy materials. In practice, it is required to provide controlled ignition with minimal energy consumption, or, conversely, to exclude the spontaneous ignition of a substance with a transition to combustion or explosion. Despite more than a century of experience in research and practice, such a task still remains relevant, and large-scale industrial disasters occur regularly in different countries.

The hot spots of ignition also play an important role in some combustion modes. It is known, at low pressures, the combustion of a propellant becomes unsteady, and the structure of the combustion wave is significantly nonuniform. Such modes are called hot-spot pulsed, with a set of hot spots that extinct and reignite and transverse combustion waves propagating along the surface of the sample [3, 4].

A qualitative analysis of the effect of surface inhomogeneity on ignition processes was carried out in the classic review by Merzhanov [6]. If the depth of the heating of the substance is comparable to the characteristic height of the surface inhomogeneities, then the uniformity of the heating of the substance is disturbed and local hot spots may arise in it. Due to self-acceleration of the chemical reaction, a positive feedback arises in hot spots, and they are additionally heated due to the chemical energy. As a result, the ignition time is noticeably reduced and the energy required to initiate the stable combustion of the entire substance is also reduced. However, expressions that quantitatively describe the ignition time in the hot spots in the general case of an inhomogeneous surface under different heating conditions remain unknown.

The problem of igniting a semi-infinite plate by an hot surface has been considered by many authors using various approximate analytical and numerical methods. The ignition of symmetric bodies of the cylinder and a sphere, as well as simple two-dimensional configurations, for example, a right angle, was also considered. A survey of these works is presented in the monographs of Vilyunov [7] and Assovskii [8].

This paper analyzes the conditions for the hot spot formation in a solid propellant of a complex geometric shape heated by a hot surface at a constant tempera-

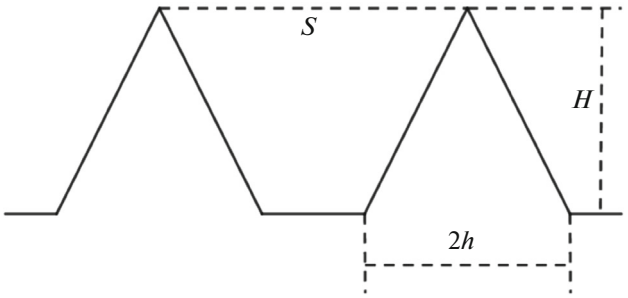

Fig. 1. Model configuration of a rough surface.

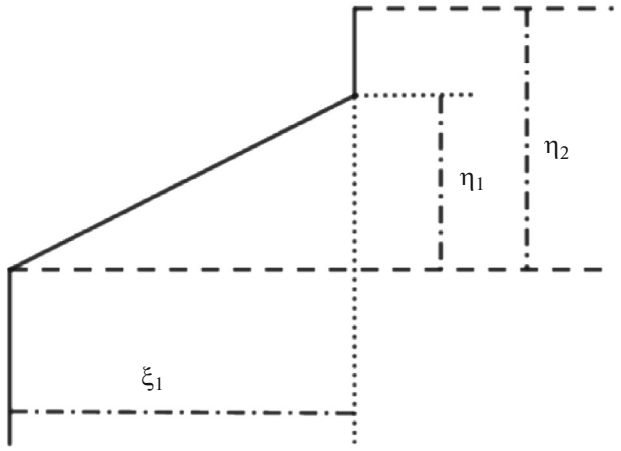

Fig. 2. A single protrusion and axes of symmetry for the computational domain.

ture. A geometrical configuration is proposed, which allows predicting the location and time of the origin of the focus. Thus, in this model, it is possible to isolate the specifics of the effect of the geometric shape of the substance on ignition and to determine the dimensionless parameters responsible for the formation of the focus.

PROBLEM STATEMENT AND MATHEMATICAL MODEL

Further in the study, the geometric configuration of the inhomogeneous surface is considered, shown in Fig. 1. This configuration simulates a rough surface composed of identical wedge-shaped ridges of the final height and final apex angle. Let us denote the height of the protrusions as H; the half-width at the base of the protrusions, as h; and the distance between the protrusions as S. The angle at the apex of the protrusion in these notation is expressed as $2\psi = 2\arctan(h/H)$.

Assume that at the moment of time $t = 0$, the temperature T_s, which is further maintained constant, is set on the surface of a substance with the initial temperature T_0. The region near the top of the protrusion warms up faster than the regions far from the top, and the chemical reaction begins precisely near the top.

In this study, the primary attention is paid to determining the dependence of the ignition characteristics on the geometric parameters, namely, on the angle at the top of the wedge, the height of the protrusion, and the distance between the protrusions. Therefore, to simulate a chemical reaction in a substance, a simple kinetic scheme of the thermal theory of ignition with a zero order of reaction is used [6].

Under the usual assumptions of the solid-phase theory of ignition, we write down the heat conduction equation with a volumetric heat source of a homogeneous chemical reaction. It follows from the symmetry of the problem that the calculations can be carried out for half of a single protrusion. Dimensionless parameters in the computational domain are shown in Fig. 2.

In a Cartesian coordinate system with the origin at the top of the wedge and the x axis directed along its axis, the wedge face is described by the equation $y = x\tan\psi$ $(0 < x < H)$. Let us write the equation for the temperature distribution in a substance in the presence of a chemical reaction in the form

$$c\rho\frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + Qz\exp\left(\frac{-E}{RT}\right) \quad (1)$$

with the following initial and boundary conditions:

$$t = 0\text{: } T = T_0; \quad (2)$$

$$0 < x < H\text{: } T(y = x\tan\psi) = T_s;$$
$$h < y < S/2\text{: } T(x = H) = T_s;$$

$$x = +\infty\text{: } T = T_0; \quad (3)$$

$$y = 0\text{: } \partial T/\partial y = 0; \quad y = S/2,$$
$$H < x < +\infty\text{: } \partial T/\partial y = 0.$$

Here T is the temperature, t is time, c is the heat capacity, ρ is the density, k is the heat conductivity, Q is the thermal effect of a chemical reaction, z is the pre-exponent, E is the activation energy, and R is the universal gas constant.

Since the problem has the characteristic temperature T_s, using the expansion of temperature according to Frank-Kamenetsky near T_s, we write the equations in dimensionless form:

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial\xi^2} + \frac{\partial^2\theta}{\partial\eta^2} + \exp\left(\frac{\theta}{1+\beta\theta}\right) \quad (4)$$

with the initial and boundary conditions

$$\tau = 0\text{: } \theta = \theta_0; \quad (5)$$

$$\begin{gathered} 0 < \xi < \xi_1\colon \theta\,(\eta = \xi\tan\psi) = 0; \\ \eta_1 < \eta < \eta_2\colon \theta(\xi_1) = 0; \quad \xi = +\infty\colon \theta = \theta_0; \\ \eta = 0\colon \partial\theta/\partial\eta = 0; \quad \eta = \eta_2, \\ \xi_1 < \xi < +\infty\colon \partial\theta/\partial\eta = 0. \end{gathered} \tag{6}$$

The following dimensionless variables and parameters are introduced: $\theta = E\,(T-T_s)/RT_s^2$ is dimensionless temperature; $\tau = t/t_{ad}(T_s)$ is dimensionless time, where $t_{ad}(T_s) = c\rho RT_s^2\exp(E/RT_s)/EQz$ is the period of induction of a thermal explosion at temperature T_s; $\xi = x/x_0$ and $\eta = y/x_0$ are dimensionless coordinates, where $x_0 = (kRT_s^2\exp(E/RT_s)/EQz)^{0.5}$; $\theta_0 = E(T_0-T_s)/RT_s^2$ is the dimensionless initial temperature; $\xi_1 = H/x_0$ is the dimensionless height of the protrusions; $\eta_1 = h/x_0$ is the dimensionless half-width of the protrusion; $\eta_2 = S/2x_0$ is the dimensionless distance between adjacent protrusions; and $\beta = RT_s/E$ is a small parameter.

The solution to system (4)–(6) is a function of time and coordinates, depending on five dimensionless parameters:

$$\theta = \theta(\tau, \xi, \eta, \theta_0, \xi_1, \eta_1, \eta_2, \beta). \tag{7}$$

In what follows, it is assumed that the dependence on β can be neglected.

System (4)–(6) was solved by numerical methods using an explicit scheme. Taking into account the assumptions made about the zero order of the reaction and neglecting the dependence on β, the ignition time τ_i and coordinates of the ignition source (ξ_i, η_i) will be functions of the corresponding dimensionless parameters:

$$\begin{aligned} \tau_i &= \tau_i\,(\theta_0, \xi_1, \eta_1, \eta_2), \\ \xi_i &= \xi_i\,(\theta_0, \xi_1, \eta_1, \eta_2). \end{aligned} \tag{8}$$

It follows from the symmetry that the ignition source is located on the axis of the wedge, i.e., $\eta_i = 0$. The task is to find these functions. In the calculations, it was possible to establish dependences describing the form of function (8) in some limiting cases.

IGNITION OF A WEDGE OF INFINITE LENGTH

A long protrusion is an important limiting case when the characteristic height of roughness noticeably exceeds the depth of heating of the bulk of the substance during the ignition time. Due to the action of the hot walls, the substance inside the protrusion quickly warms up. After some time, a hot spot appears near the vertex, in which the temperature begins to increase rapidly and in finite time tends to infinity. Due to the fact that the walls' temperature is constant, this spot develops in the depth of the substance at a certain distance from the surface. As soon as the maximum temperature in the hot spot exceeds the surface temperature, heat flows into the walls, which turn from a heat source into a heat sink, and the hot spot begins to migrate into the interior of the substance. Due to symmetry, the center of the hot spot is always located on the axis of the wedge-shaped protrusion, but drifts inward from the top. For a protrusion of sufficiently large length (i.e., in dimensionless form, $\xi_1 \gg 1$ and $\eta_1 \gg 1$), the presence of a cold base does not affect the temperature distribution, and functions (8) can be written as $\tau_i = \tau_i\,(\theta_0, \psi)$ and $\xi_i = \xi_i\,(\theta_0, \psi)$, where $\tan\psi = \eta_1/\xi_1$.

The numerical calculations revealed an exponential dependence of the ignition time on the angle at the vertex of the protrusion in a wide range of its values, $10° < 2\psi < 150°$. This dependence can be approximated by the following formula:

$$\tau_i = f\,(|\theta_0|)\exp[g\,(|\theta_0|)\,\psi], \tag{9}$$

where angle ψ is expressed in degrees, and the functions $f(x)$ and $g(x)$ have the form

$$f(x) = 2.6 + 0.14x - 0.0076x^2 - 0.001x^3,$$

$$g(x) = 0.0056 + 0.0028x - 5\times10^{-6}x^2.$$

In the estimates, it can be assumed that the ignition time $\tau_i \backsim |\theta_0|^{4\psi/\pi}$. Note that this formula gives the correct quadratic dependence of the ignition time on the initial temperature also for a flat surface ($2\psi = \pi$): $\tau_i \backsim |\theta_0|^2$. The sharp exponential dependence of the ignition time on angle ψ is related to the fact that the protrusion is heated much faster than in the one-dimensional case. For a flat surface in a one-dimensional mode, ignition requires the creation of a heated layer of sufficient depth and the time of inert heating strongly depends on the initial temperature. In the protrusion, a chemical reaction is initiated immediately on exposure to hot walls, and a focus arises where the dimensionless temperature is greater than zero. In this case, the ignition time of the hot spot is determined by how quickly its size reaches a value of the order of unity (in our dimensionless parameters), after which a thermal explosion of the hot spot occurs.

The calculations revealed that the center of the hot spot is located at an approximately constant distance from the wall at the moment of ignition, regardless of the angle and initial temperature. Thus, the location of the hot spot can be accurately predicted by determining on the axis of the protrusion the point for which the distance from the wall of the protrusion is ≈ 1.5. Note that the value is very close to the one determined earlier in our work on the thermal explosion of bodies of arbitrary shape [9].

For very small angles ($2\psi < 10°$), the ignition time tends to a constant value: $\tau_i = 3$–4, and actually does not depend on the initial temperature of the substance. This mode corresponds to the ignition of a layer of substance heated from both sides by hot plates.

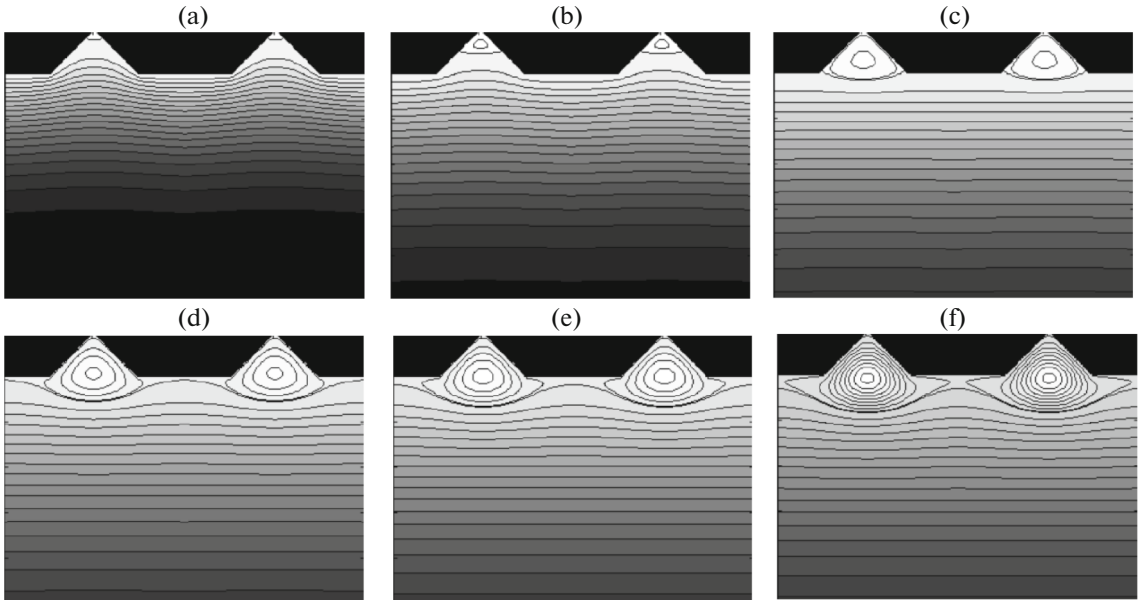

Fig. 3. Penetration of the hot spot deep into the substance: (a) inert heating; (b) the emergence of a hot spot near the vertex; (c–e) migration of the hot spot into the interior of the substance; (f) the final position of the hot spot.

IGNITION OF SMALL ROUGHNESSES

In another important limiting case, the characteristic height of roughness is smaller than the depth of the heating of the bulk of the substance during the ignition time. In this case, the ignition time tends to the value of the ignition time of a flat surface. However, the presence of roughness disturbs the uniformity of the temperature distribution along the axis of the substance and plays the role of a perturbing factor for solving the heat conduction equation in the presence of a chemical source. The term related to the chemical source depends on temperature exponentially, while the characteristic parameters of the diffusion term in the heat equation depend on temperature in a power-law manner.

Therefore, even in the presence of small surface roughnesses, the ignition of the substance occurs in separate hot spots. If both the height of the protrusions and the characteristic distance between them are much smaller than the characteristic size of the hot zone (i.e., much smaller than unity in our dimensionless parameters), then these hot spots subsequently merge and form a single combustion wave. In practice, as a rule, the nonuniformity of the surface is combined with uneven heating, and it is extremely difficult to achieve the uniform ignition of a substance over the entire surface. In the case of heating by an external heat flux, the presence of surface roughness leads to the fact that the effective surface of interaction with an external source increases and the heat flux into the substance also increases.

PENETRATION OF THE HOT SPOT UNDER THE SURFACE OF THE SUBSTANCE

When the characteristic height of the protrusions is equal in order of magnitude to unity, the hot spots penetrate deep into the substance. Figure 3 shows the results of the numerical calculations for the following parameter values typical for ignition problems: the initial temperature $\theta_0 = -10$ and the square angle at the vertex of the protrusion with height $\xi_1 = \eta_1 = 2$.

The calculations revealed that the hot spots penetrate deep into the substance, but do not merge with each other. In the course of the development of the hot spot, the following stages can be distinguished. At the stage of inert heating (Fig. 3a), the thermal boundary layers from the walls of the wedge are closed in the region of the apex, where the nucleus of the hot spot is formed—a small area with a temperature in the center higher than the temperature of the walls. In Fig. 3a, this area is almost invisible, but it gradually moves along the axis of the protrusion towards the bulk of the substance, increasing in size (Figs. 3b, 3c). The maximum temperature in the hot zone also increases; however, due to the proximity of the walls, ignition in the nucleus of the hot zone is impossible as long as it is at a distance less than the critical distance from the walls.

When the center of the hot spot moves away from the walls at a distance of more than one, the temperature in the center of the hot spot rises rapidly and it ignites (Figs. 3d, 3e). The distance from the center of the ignition to the nearest point of the wall is practically independent of the initial temperature and geometric parameters and is always ≈1.5 in our dimensionless variables.

The experiments show that, after ignition in the hot spot, the modes of the developed combustion wave substantially depend on the external conditions. At high pressures, the reactions in the gas phase play a significant role: the zone of an intense chemical reaction is located close to the surface and makes a significant contribution to the heat balance at the surface. Thus, the combustion wave is supported by an external heat source and propagates in the form of a uniform front. At low pressures, the relative role of heat release in the condensed phase increases, and the one-dimensional front loses its stability and breaks down into a set of extinguishing and igniting spots and transverse combustion waves.

DISCUSSION AND CONCLUSIONS

As noted earlier and in our work on the study of thermal explosion in bodies of an arbitrary shape [9], when a substance is ignited by a heated surface at a constant temperature, the surface itself from a heat source turns into a sink as soon as the temperature inside the substance becomes higher than the surface temperature. The hot spot formed under the surface of the substance moves away from the surface until the parameters of the spot become sufficient for a spontaneous thermal explosion by the Merzhanov mechanism [10].

It should be emphasized that when a substance is ignited by a hot surface, even small inhomogeneities of the latter perturb the one-dimensional temperature distribution and lead to the formation of hot spots. The determining factor for this behavior of the reactive substance is the strong exponential dependence of the reaction rate on temperature. In spite of the fact that the surface is a heat sink for a source that has arisen in the depth of the substance, it is not able to prevent ignition if the source migrates into the depth of the substance at a distance of the order of unity in our dimensionless coordinates. The hot spot develops in the thermal explosion mode, and its ignition occurs during the time of the order of one period of the thermal explosion of the substance at the given temperature, since the reaction term in the heat balance equation clearly dominates the diffusion term.

This mechanism can play an important role in the so-called hot-spot pulsed modes of combustion of solid propellant [11]. In our work [12], it is shown that in the presence of heat loss from the surface of a substance, a pulsating mode of the combustion of a propellant can occur due to the instability of the combustion of the subsurface layer by the mechanism of thermal explosion. The combustion front propagates at a variable speed, and the characteristic size of the front pulsations is determined by the width of the reacting layer in the condensed phase and increases with decreasing surface temperature. The frequency of the pulsations is inversely proportional to the time of the adiabatic thermal explosion of the hot spot arising under the surface of the substance. A description of such a nonstationary combustion mode is beyond the scope of this article and requires the accumulation of experimental data and the development of the corresponding multidimensional models.

Thus, it is shown in this study that the presence of protrusions and surface roughness can cause the formation of ignition hot spots. Dimensionless parameters are found that characterize the ignition time of the hot spot and the location of a hot spot in the substance.

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