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Theoretical Analysis on the Hot Surface Ignition of a Rectangular-Shape Solid Fuel

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Abstract—Ignition of a reactive solid in a shape of square corner by a hot surface is studied theoretically. Ignition time and the location of ignition point are determined as a function of dimensionless parameters, with the use of the homogeneous model of ignition. The effect of geometry on the ignition of solid fuel results in the local characteristics: the reaction is initiated in a hot point in depth of the substance. It is shown that ignition time is proportional to the dimensionless initial temperature, whereas for the ignition of the semiinfinite body this dependence was quadratic.

1. Introduction

Ignition and flame spread over solid fuel is a basic problem in the field of solid propellant propulsion and fire research. To ignite a solid fuel, an external thermal stimulus is required, and under the action of this stimulus the upper layers of the solid fuel are heated and exothermic reactions are accelerated. Any cold part of the solid fuel that is remote from its surface acts as a thermal energy sink. Ignition occurs only when the heat release rate in the chemical reaction zone becomes either equal to or higher than the heat loss rate. In some cases heat losses are possible not only to the depth of the solid fuel but also to the ignition medium. Extensive reviews of research works performed in this area were conducted by Kulkarni *et al.*[1] and Price *et al.*[2], and excellent summary on solid propellant ignition theories and experiments is also given by Hermance[3].

Previously, researchers developed the modern theory of ignition of reactive solids for the one-dimensional modeling of ignition of regular-shaped bodies such as semi-infinite body, cylinder or ball[4-9]. However, much experimental evidence exist about the multidimensional character of ignition process. That is, it is generally known that the chemical reaction is primarily initiated at hot spots, which, in turn, ignite the whole substance[1,3,9-11].

Recently, some efforts have been done to evaluate the effect of geometry on ignition, because the surface irregularities, that is, the presence of protrusions, sharp edges, might be a favorable condition for appearing the hot spots, or the initiation of ignition. Vorsteveld and Hermance[5,10] considered the ignition of wedge by a constant heat flux and found, that the ignition delay was decreased 3.6 times for a square-angle wedge, and even more for the acute angles, compared to the ignition delay of the semi-infinite body.

In this paper the ignition of the square-angle of the solid fuel plate by hot surface is considered. Two-dimensional thermal theory model of a solid fuel ignition is developed using homogeneous model of ignition. The ignition delays are calculated, and the local characteristic of ignition of solid fuel are discussed.

2. Mathematical Model Formulation

The square angle of a reactive solid fuel plate with the initial temperature To is considered as the model geometrical configuration. A schematic diagram of the model is shown in Fig. 1. Temperature varies in the x(ξ) and y(μ) directions. The surface of square angle is exposed to high surface temperature T* and maintained constant during the whole process. It is assumed that the one-step irreversible chemical reaction can occur in the substance. The reaction rate W(T) is described by the Arrhenius expression: $W(T)=Z\exp(-E/RT)$. In this model, reactant depletion effect is

neglected, which is correct for the homogeneous model of ignition. That is, the solid phase reactions are of zero order with respect to reactant concentration, and the ignition time is so short that the solid fuel consumption is negligible. It is beneficial, in general, to neglect the reactant depletion in this type of ignition problems, because when the depletion is important, the ignition process becomes degenerated, and the solid-phase ignition model is no longer valid. In this paper we pay attention primarily to the effect of geometry on ignition.

Mathematical formulation of the problem is given by energy equation for temperature distribution along with initial and boundary conditions.

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \frac{QZ}{c}\exp\left(\frac{-E}{RT}\right) \tag{1}$$

Initial and boundary conditions:

$$T = t(t,x,y): \quad t>0,\ x,y>0$$

$$T(0,x,y) = T_o;\ T(t,0,y) = T^*;\ T(t,x,0) = T^*;$$

$$\partial T(t,\infty,y)/\partial x = \partial T(t,x,\infty)/\partial y = 0 \tag{2}$$

In Eq.(1) and (2), the variables are defined as follows: T=temperature; t=time; x and y=cartesian coordinates; a=thermal diffusivity; Q=heat of reaction; Z=preexponential factor; c=specific heat; r=density; l=thermal conductivity; E=activation energy; R=universal gas constant; T0=initial temperature; T*=temperature of the hot wall.

To solve the above equation along with initial and boundary conditions, it is essential to transform the variables into dimensionless forms. By using new variables appropriate for a given problem, one can readily estimate the role of dimensionless terms and thus reduce the number of parameters. Within the framework of the solid-phase ignition theory[4] proposed by Frank-Kamenetsky, the governing equation and intial and boundary conditions are transformed into dimensionless form. The resulting dimensionless form are written down as follows:

$$\frac{\partial\theta}{\partial T} = \frac{\partial^2\theta}{\partial\xi^2} + \frac{\partial^2\theta}{\partial\eta^2} + \exp\left(\frac{\theta}{1+\beta\theta}\right) \tag{3}$$

Initial and boundary conditions:

$$\theta = \theta(\tau,\xi,\eta), \quad \tau>0,\ \xi,\eta>0$$
$$\theta(0,y,\phi) = \theta_0;\ \theta(u,+\infty,\phi) = \theta_0; \tag{4}$$
$$\partial\theta(\tau,\infty,\eta)/\partial\xi = \partial\theta(\tau,\xi,\infty)/\partial\eta = 0$$

Dimensionless variables and parameters:

$$\theta = E(T-T^*)/RT^{*2};$$
$$\xi = x/r_0;\ \eta = y/r_0;$$
$$\tau = t/t_0; \tag{5}$$
$$r_0 = \lambda RT^{*2}/qE; t_0 = r_0^2 c\rho/\lambda;$$
$$\theta_0 = E(T_0-T^*)/RT^{*2};\ \beta = RT^*/E$$

In Eqs. (3), (4), and (5), the variables are defined as follows: t_o, r_o=time and space coordinate characteristic scales; θ=dimensionless temperature; τ=dimensionless time; xi, η=dimensionless space coordinates.

The solution of governing equation (3) and boundary condition (4) depends on two dimensionless parameters: θ_o, dimensionless initial temperature, and β-the small parameter which shows the strength of the temperature dependence of the reaction rate. The effect of parameter b is usually negligible in ignition problems, if the Frank-Kamenetski's expansion of the exponent is performed based upon the ignition scale temperature T*[7]. In addition, Frank-Kamenetski's parameter is of no importance for the ignition problem[6]. Thus the critical ignition condition suggests the following form.

$$\tau^* = \tau^*(\theta_o, \beta) \tag{6}$$

where τ^* is the critical time of the solid-phase heating. Generally, the characteristic values of θ_0 in the ignition problems range from -5 down to -25; the value of b is typically 0.02-0.03.

The physical meaning of the new time and distance scales is as follows. The quantity to is the adiabatic induction period. If the whole body of solid fuel is instantly heated up to the hot temperature T* inside an adiabatic envelope, the reaction time of the system is determined by t_o. The meaning of r_o becomes clear; it determines the order of the heating zone width of the solid phase within the adiabatic induction period.

Due to the strong dependence of chemical reaction rate on temperature, at the first stages of heating the substance is not heated enough for the chemical reaction to occur at the significant rate. As the temperature is increased, the chemical reaction is in-

itiated, and the chemical heating also comes into effect. Approaching the ignition moment, $\tau \rightarrow \tau^*$, the temperature in the ignition point (ξ^*, η^*) will increase drastically, and for β=0 will asymptotically tend to infinity:

$$\theta(\tau \rightarrow \tau^*, \xi^*, \eta^*) \rightarrow \infty \tag{7}$$

The purpose of this work is to determine the ignition time and the ignition coordinates as the functions of the dimensionless parameters:

$$\tau^* = \tau^*(\theta_o, \beta); \quad \xi^* = \xi^*(\theta_o, \beta); \quad \eta^* = \eta^*(\theta_o, \beta) \tag{8}$$

3. Numerical Method

To obtain the dependencies of Eq. (8), the governing equation, Eq. (3), was numerically integrated. The explicit finite-difference method is applied. The time derivative was approximated by a first-order forward difference expression, whereas second-order central difference expressions were used for the spatial derivatives. After the discretization, the equation for the temperature in the node (k, j) at the next time step (n+1) is expressed in finite difference form as follows.

$$\theta_{k,j}^{n+1} = (1-4*\mathrm{Fo})\cdot\theta_{k,j}^{n} + \mathrm{Fo}\cdot(\theta_{k+1,j}^{n} + \theta_{k-1,j}^{n} + \theta_{k,j-1}^{n} + \theta_{k,j+1}^{n}) + d\tau\cdot\exp(\theta_{k,j}^{n}), \tag{9}$$

where $\mathrm{Fo}=d\tau/d\xi^2$ is the Fourier number.

The known analytical solution for the temperature distribution in the absence of the chemical heating was used to check the consistency of the numerical scheme. For the uniform grid with equal spatial steps along the ξ and η coordinates, the choice of Fo=1/6 allows to achieve accuracy of the order $O(d\tau^2, d\xi^4$ (for the inert scheme). The limits of the stability are: $0<\mathrm{Fo}\leq 0.25$.

4. Results and Discussions

Qualitatively, the solution behaviour can be described as follows. Immediately after the beginning of heating, the hot zone is formed in the region of the corner, due to the strong double-side heating by the hot walls. The thermal waves from both sides of the corner propagate into the depth of the substance as shown in Fig. 2. Thus, it results in the temperature rise and initiation of the chemical reaction. After some induction period, when the heat supply is sufficient for the chemical reaction to begin, the hot spot is formed at the some distance from the angle vertex. This phenomena is shown in Fig. 3. Since the temperature of the walls is less than the temperature of the hot spot, the walls become the heat sink in the region of the vertex, and the hot spot drifts into the depth of the substance, its maximal temperature rising with time. When the heat balance between the

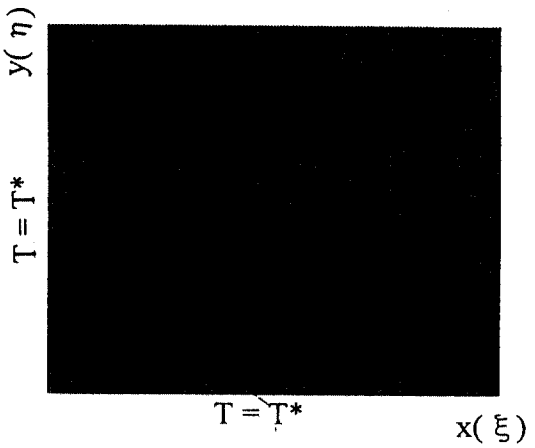

Fig. 1. The schematic diagram of the model: ignition of square angle by hot surface.

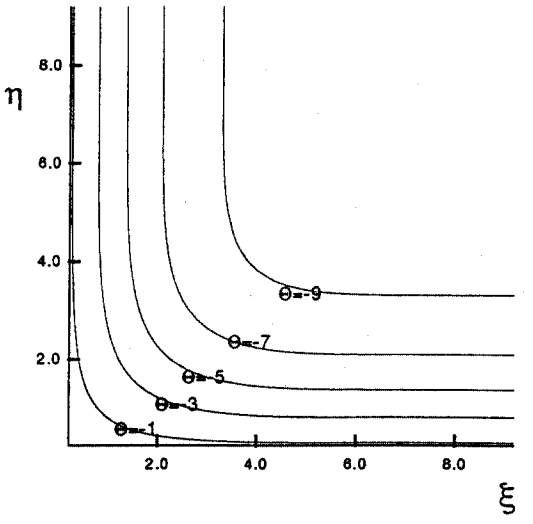

Fig. 2. Tehmperature distribution inside the square angle.Θ_o=-10; τ=2.0.

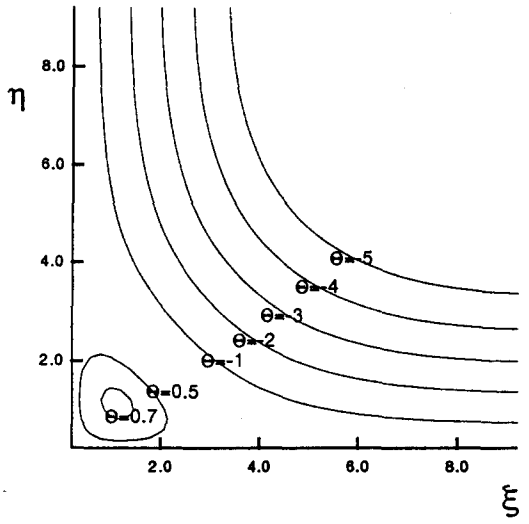

Fig. 3. Temperature distribution inside the square angle. Θ_o=-10; τ=10.0

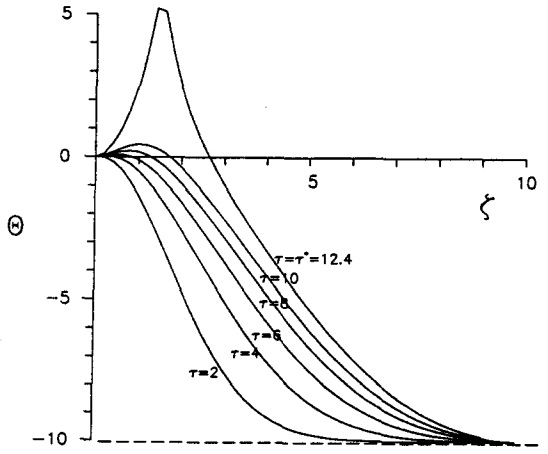

Fig. 4. Temperature distribution along the centerline as a function of time; Θ_o=-10.

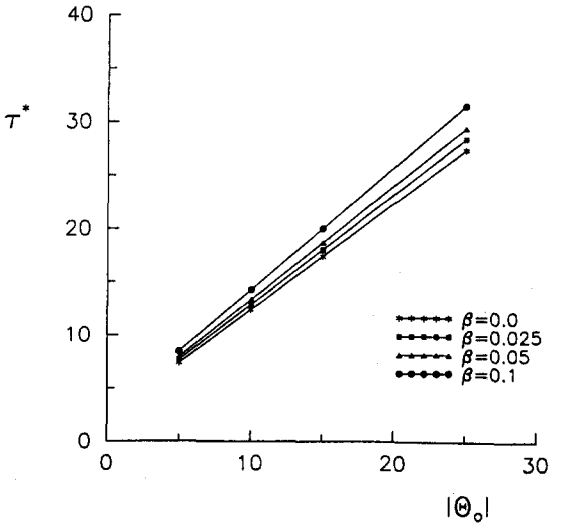

Fig. 5. Effects of initial temperature on ingnition delay for varying β.

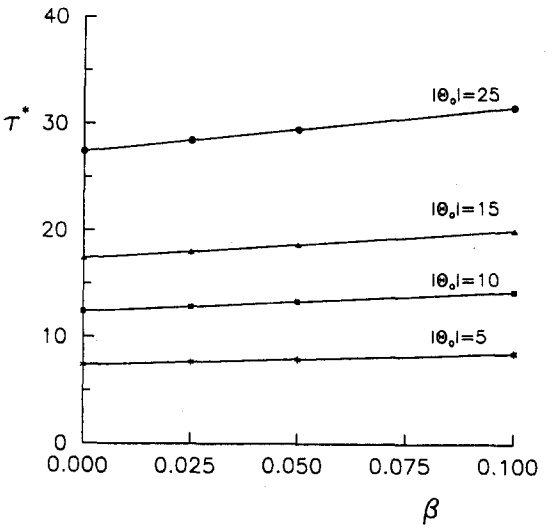

Fig. 6. Effects of β on ignition delay for varying initial temperature.

heat generation by the self-accelerating chemical reaction and heat loss by conduction cannot be further maintained, the thermal runaway occurs, and the substance is ignited. The temperature distribution evoluting with time along the center line $\xi=\eta$ is shown in Fig. 4., where one can notice the propagation of the appearing hot spot into the depth of the substance. The temperature overshoot in the figure at τ=12.4 clearly indicates the initiation of ignition at that spot. That is, the ignition starts at time τ=12.4 and at the space coordinate $xi=\eta$=1.4 at the given condition; θ_o=-10 and β=0.

The effects of initial temperature (o and b on ignition delay are analyzed for wide ranges of the two parameters, and the results are shown in Figs. 5 and 6. It is evident from Fig. 5 that the ignition delay varies linearly with θ_o. Fig. 6 shows the effect of β on ignition delay. It can be found the fact that b affects ignition characteristics only slightly.

The numerical calculation is performed for the

whole ranges of θ_o and β to obtain the evolution of the temperature θ. In addition, from the analysis of the temperature profile the ignition delay and the ignition coordinates, τ^*, ξ^*, η^*, are determined. The results are tabulated in Table 1. It can be seen that τ^* is affected greatly by θ_o, but it is affected weakly by β. It is clear from the table that the ignition coordinate is almost constant for the whole ranges of calculations. That is, the ignition coordinate is independent of θ_o and β. However, it should be noticed that the dimensional ignition coordinate x* (y*) is not a constant but varies with T*.

Using the results of numerical calculations, a multiple least square regression method is used to correlate the ignition delay and the ignition coordinates to the two independent variables; θ_o and β.

A correlation equations for ignition delay is obtained from the results of numerical calculations. The results of the approximation is represented by the following equations:

Ignition delay ($5 < |\theta_0| < 25$, $0 \le \beta \le 0.1$):

$$\tau^* = (|\theta_0| + 2.4)*(1+1.5\beta) \quad (10)$$

Ignition coordinates:

$$\xi^* = \eta^* = 1.4 \quad (11)$$

For the one-dimensional case, the ignition delay is determined by the following equation[9]:

Table 1. Results of calculatios on ignition delay and ignition coordinates.

β	$\|\theta_0\|$	τ^*	$\xi^*=\eta^*$
0.000	5	7.39	1.39
	10	12.41	1.39
	15	17.40	1.40
	25	27.42	1.41
0.025	5	7.69	1.39
	10	12.87	1.39
	15	18.03	1.40
	25	28.46	1.41
0.050	5	7.94	1.40
	10	13.35	1.40
	15	18.69	1.41
	25	29.47	1.42
0.100	5	8.50	1.39
	10	14.27	1.40
	15	20.02	1.41
	25	31.54	1.41

$$\tau^*_{1D} = (0.165 \cdot \theta_0^2 + 2|\theta_0| + 1) * (1+\beta) \quad (12)$$

The ignition delays of the semi-infinite body and the square angle, that is the delay times of one-dimensional and two-dimensional cases are presented in Figs. 7 and 8. It is evident from the figure that the ignition delay in two-dimensional case is reduced significantly, compared to the one-dimensional case, by the factor of 2.5-5, depending on the dimensionless initial temperature. The functional dependence of the ignition delays is also affected by the geometry: the ignition delay is proportional to the first power of the dimensionless initial temperature for the two-dimensional case, whereas the dependence for the one-dimensional case is quadratic. Therefore, the convergence of the temperature waves, propagating from the both sides of the corner, supplies the heat suf-

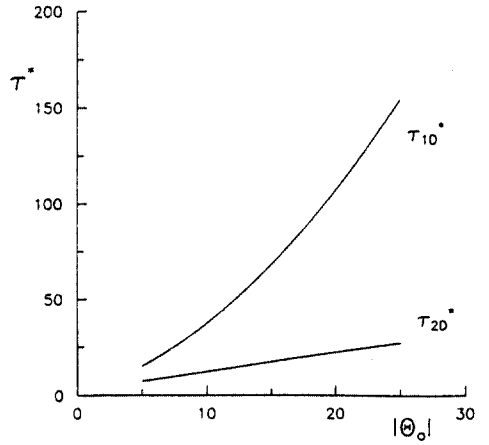

Fig. 7. Effect of initial temperature on ignition delays.

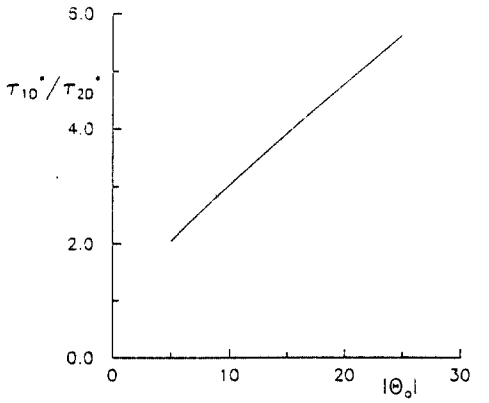

Fig. 8. The ratio of ignition delays for the 1-D and 2-D cases as a function of initial temperature.

ficient to quickly ignite the substance locally, at the ignition point, whereas in the case of ignition of smooth surface, much more time is required to accumulate heat in the layer, adjacent to the surface.

The location of the ignition point turned out to be insensitive to the variations of the initial temperature. The value of ξ^* is very close to the reported values for the one-dimensional case: $\xi^* = 1.37$[4].

From Eq. 10, the dimensionless ignition delay can be expressed into dimensional form using the relation defined in Eq. 5. The ignition delay of the square angle in dimensional units is expressed as follows:

$$t^*_{2D} = (2.4+E(T^*-T_0)/RT^{*2})$$
$$(1+1.5RT^*/E)\lambda c\rho RT^{*2}\exp(E/RT^*)/EQZ \qquad (13)$$

One can notice the strong exponential dependence of the ignition delay upon the activation energy E and the hot wall temperature T^*. The dependence on other parameters is not so pronounced.

5. Conclusions

The present research provides an estimation of ignition characteristics of surface shape. Ignition time and the location of ignition point were determined as a function of dimensionless initial temperature and small parameter β. It is found that at the time of initiation of ignition the hot spot is formed at some distance from the vertex, and sudden rise of temperature at that point can be observed. That is, the effect of geometry on the ignition of solid fuel results in the local characteristics: the reaction is initiated in a hot point in depth of the substance.

Ignition delay is proportional to the first power of the dimensionless initial temperature, whereas for the ignition of the semi-infinite body this dependence was quadratic. It is found that ignition delay shows the strong exponential dependence on the activation energy and hot wall temperature. The location of the ignition point does not depend on the dimensionless initial temperature.

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