LASER-INDUCED IGNITION OF REACTIVE SOLIDS WITH ROUGH SURFACE

Jae-Ou Chae*, Gregory N. Mokhin**, Nam-Ki Kim*

* Dept. of Mechanical Engineering, INHA Univ., Inchon;
** N.N.Semenov Inst. of Chemical Physics, Russian Acad.Sci., Moscow.

ABSTRACT

Ignition of a reactive solid with rough surface by constant heat flux is studied. The geometry of surface is represented by a protrusion in shape of cone of infinite length. Ignition time and ignition criterion versus apex angle are determined, with the use of heterogeneous model of ignition. To study the effect of geometry on ignition the results are compared with the known results for the one-dimensional ignition of the semi-infinite body. It is shown, that: a) ignition time depends strongly upon the apex angle and is proportional to the angle to the second power; b) ignition criterion and ignition temperature do not depend strongly on angle. The ignition delay and the energy required for the successful ignition are substantially reduced compared to the one-dimensional case.

INTRODUCTION

Ignition of reactive solids by a laser source often begins locally, with the initiation of the chemical reaction in a hot point. Such a hot point, or a leader of ignition is formed in the region where the intensity of heat flux is maximal so the substance gets heated up locally to a relatively higher temperature, and the conditions for the initiation of the chemical reaction are the most favorable. Among the possible causes for the local initiation, one can note the non-uniformity of the heat flux, the heterogeneity of the solid substance, as it is the case for the composite propellants, or the complexity of the surface geometry, which is the subject of the main interest in this paper. When protrusions, sharp edges, roughness and the like irregularities are present on the surface of the solid, the conditions of heat transfer are the

most favorable namely at these irregularities. Whatever factor is dominant, as a result the temperature distribution in the solid phase becomes multidimensional, and the characteristics of ignition will differ from those for the substance with the smooth surface.

It is well known, that the ignition delays, depending upon the intensity of the heat flux incident on the surface, can vary greatly, from seconds to milliseconds. For the typical values of heat conductivity of solid propellants, $\alpha \approx 10^{-3}$ cm^2/s, the penetration depth of the thermal wave for the ignition delays t* of the order of magnitude of 10^{-3} s would be equal to $d \approx (\alpha t^*)^{0.5} = 10^{-3}$ cm. The value of the characteristic thickness of the reacting layer, where the chemical reactions occur, would be even smaller. For such small values of the heated layer, usually the surface of propellants should be considered as rough. Since the multidimensionality of the heat transfer is the key feature of this type of problems, their adequate treatment requires the development of the multidimensional ignition theory. The adequate treatment of this type of problems requires the development of the multidimensional ignition theory.

However, the modern ignition theory has been developed for the modeling of one-dimensional ignition of regular-shaped bodies such as semi-infinite body, cylinder or ball [1,2]. However, multidimensional ignition problems have been investigated until now only in few publications. By means of direct two-dimensional numerical integration of the solid-phase governing equation, Vorsteveld and Hermance [3,4] considered the ignition of a wedge by constant heat flux applied to the surface and found, that the ignition delay was decreased 3.6 times for a square-angle wedge, and even more for some acute angles considered, compared to the ignition delay of the semi-infinite body. Margolin, Mokhin and Krupkin [5-7] studied the ignition of acute wedges and cones. In their papers, the analytical two-dimensional solutions of the inert (without chemical reaction) heating of wedge and cone were obtained and utilized for the analysis of the ignition in the whole range of angles. For the very acute angles, the method of temperature averaging was developed, because this problem is too difficult for the direct numerical solution, and the ignition characteristics were found as a function of the apex angle and other parameters. The configurations considered by now do not represent fully the geometry of real surface, where the protrusions are of finite height.

In the present paper the ignition of reactive solids by a constant heat flux provided by a laser source is studied.

Protrusions of the surface are modeled as an infinite cone with an arbitrary apex angle. Heterogeneous ignition model [1,2] is used, and the temperature-averaging technique is applied for the treatment of the small apex angles. The ignition characteristics, such as ignition delay, ignition criterion and ignition temperature are found as a function of apex angle.

Problem Formulation

A diagram of the model is shown in Fig.1. An infinite cone with apex angle $2\varphi_0$ is considered as a model geometrical configuration. Constant heat flux of intensity q provided by laser source is exposed to a surface. In case of ignition by laser, the normal component of the heat flux depends on the apex angle of the protrusion and is equal to $q \sin\varphi_0$. The dependence of the value of heat flux on the orientation factors is the important feature of the ignition by laser source, and previous researches [3-7] did not take it into account. One-step, irreversible heterogeneous reaction between the solid-phase fuel and the ambient oxidizer can take place on the surface. The temperature dependence of the reaction rate W(T) is described the reaction rate by the Arrhenius law: $W(T) = Z\exp(-E/RT)$. It provides additional heat flux, heating the substance, which intensity is presented as follows [2]:

$$q_{ch} = (\rho_g Y)^{\mu} Q Z \exp(-E/RT),$$

where ρ_g - is the oxidizing gas density, Y - oxygen mass fraction, μ - the factor, describing the order of the heterogeneous chemical reaction. The other values are explained in the Nomenclature.

Mathematical formulation of the problem is given by energy equation for temperature distribution along with initial and boundary conditions. Within the framework of the heterogeneous ignition theory [1,2], the reaction depletion being neglected, the governing equations in dimensional form are written down as follows:

$$c\rho\frac{\partial T}{\partial t} = \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r} + \frac{1}{r^2\sin\varphi}\frac{\partial}{\partial\varphi}\left(\sin\varphi\frac{\partial T}{\partial\varphi}\right)\right) \quad (1a)$$

Initial and boundary conditions:

$$T = T(t, r, \varphi);\ t > 0;\ r > 0;\ 0 < \varphi < \varphi_0$$

$$T(0, r, \varphi) = T_0; T(t, \infty, \varphi) = T_0; \quad (1b)$$

$$\frac{\lambda}{r}\frac{\partial T}{\partial r}(t, r, \varphi_0) = q + q_{ch};$$

$$\frac{\partial T}{\partial r}(t, r, 0) = 0.$$

The introducing the dimensionless variables merits more specific consideration,

because in the case of ignition by heat flux, contrary to the ignition by a hot surface of constant temperature, we do not know the temperature in the reaction zone, to be used as the predetermined ignition scale temperature. It is commonly accepted, that the Frank-Kamenetsky expansion of the exponent [8], with the dimensionless temperature θ defined as $\theta=E(T-T^*)/RT^{*2}$, would significantly simplify the problem. Therefore, we will use this expansion with the post-determined scale temperature T*, that is the value of T* is to be determined in course of the solution. For the dimensionless scales for time and the coordinates we have:

$y = r / r_0$; $u = t / t_0$; where $r_0 = \lambda RT^{*2}/qE$; $t_0 = r_0^2 c\rho/\lambda$.

So, the governing equations and initial and boundary conditions are rewritten in the dimensionless form as follows:

$$\frac{\partial\theta}{\partial u}=\frac{\partial^2\theta}{\partial y^2}+\frac{2}{y}\frac{\partial\theta}{\partial y}+\frac{1}{y^2\sin\varphi}\frac{\partial}{\partial\varphi}\left(\sin\varphi\frac{\partial\theta}{\partial\varphi}\right) \qquad (1'a)$$

$$\theta=\theta(u,y,\varphi);\ u>0,\quad y>0,\quad \varphi<\varphi_0$$

$$\theta(0,y,\varphi)=\theta_0;\quad \theta(u,+\infty,\varphi)=\theta_0;$$

$$\frac{1}{y}\frac{\partial\theta}{\partial\varphi}(u,y,\varphi_0)=1+\Omega\exp\left(\frac{\theta}{1+\beta\theta}\right);$$

$$\frac{\partial\theta}{\partial\varphi}(u,y,0)=0.$$

Four dimensionless parameters, along with φ_0, appear after non-dimensionalization:

$\theta_0=E(T_0-T^*)/RT^{*2}$; $\Omega = (\rho_g Y)^{\mu}QZ\exp(-E/RT)/q$; $\beta = RT^*/E$.

Frank-Kamenetski's expansion of the exponent based on the post-determined ignition scale temperature T* allows to minimize the dependence on small β-parameter, which otherwise should have been taken into account. Therefore, from the analysis of dimensionless parameters we can conclude, that the temperature distribution and solution behaviour would be a function of three dimensionless parameters: $\theta = \theta(u, y, \varphi, \theta_0, \Omega, \varphi_0)$, the ignition criterion will be determined from a relationship between the dimensionless parameters: $\Omega^*=\Omega^*(\theta_0, \varphi_0)$; and the ignition time will read as follows: $u^*=u^*(\theta_0, \Omega^*, \varphi_0)$.

Analysis of the Inert Heating

We have obtained the analytical solution of inert problem (system (1'), Ω=0), describing the temperature distribution due to the heating by external source, without chemical reaction. Since the full form of the solution is rather complex, its explicit expression is presented in Appendix 1. The

equation for the cone apex temperature as a function of time and the angle is as follows:

$$\theta(u, 0, 0) = \theta_0 + B\, u^{0.5},$$

where $B = 2\pi^{-0.5} \tan^{-1}(0.5\varphi_0)$.

Due to strong dependence of chemical reaction rate on temperature, chemical heating comes into effect right before the ignition moment. The ignition time can be preliminary estimated as the time required for inert heating of the body up to the ignition temperature T*, independently of the actually employed ignition theory. Therefore, with the use of the analytical solution, the dimensional ignition time can be estimated preliminary as follows:

$$t^*_{2D} = \frac{\pi}{4} \frac{\lambda c \rho \left(T^*(\varphi_0) - T_0\right)^2}{q^2} \tan^2\left(0.5\varphi_0\right) \quad (2)$$

One can notice that this equation gives the well-known result for the ignition of the semiinfinite body, when $\varphi_0=\pi/2$. The equation (2) is directly applicable for the quantitative estimation of ignition time, if the value of T* is determined in one or another ignition model. However it provides qualitatively correct dependence of ignition time on angle, no matter what key steps of chemical reaction are involved, because T* is much less dependent on φ_0.

The Treatment of the Small Angles: Temperature Averaging Method.

For the treatment of the small angles direct numerical integration of (2) is not possible, and we take the advantage of the method of temperature averaging upon the isotherms, developed in our previous studies [5-7]. For the thin body, the thermal boundary layers in the region of the apex converge, and the heat transfer occurs mainly in the radial (r) direction, while in the angular (φ) direction it can be neglected. The isotherms are approximately represented by the equation r = const, that is T=T(r), the dependence on φ is small, and the temperature may be averaged along the isotherms. The procedure of temperature averaging gives correct results for the small angles φ_0, and moreover, in [5] it was proved, that for the infinitely long wedge the results remain valid in the whole range of angles $0<\varphi_0<\pi/2$. It allows to reduce the number of variables and parameters, as well as to find the functional relationships among the system parameters in the limit case of small angle φ_0.

Upon performing averaging of the temperature: $\overline{\theta} = \int_0^{\varphi_0} \theta \sin\varphi \, d\varphi \,/\, (1-\cos\varphi_0)$, the averaging symbol will be omitted) and introducing new dimensionless scales, the equation for temperature distribution in the

thin cone along with initial and boundary conditions is as follows:

$$\frac{\partial\theta}{\partial\tau}=\frac{\partial^2\theta}{\partial x^2}+\frac{2}{x}\frac{\partial\theta}{\partial x}+\frac{2}{x}(1+\Omega\exp\theta) \quad (3)$$

$\theta = \theta(\tau, x); \quad 0 < x < \infty; \quad \tau > 0;$

$\theta = \theta(0, x) = \theta = \theta(\tau, \infty) = \theta_0;$

$$x\frac{\partial\theta}{\partial x}(\tau, x\to 0)=0,$$

where $x = r/r_1$, $\tau = t/t_1$, $t_1 = c\rho r_1^2/\lambda$; and $r_1 = 2r_0\tan(0.5\varphi_0)$. It is evident, that due to the temperature averaging the dependence on angle φ_0 is incorporated into the dimensionless variables and parameters.

The analytical solution of system (3) for the case of inert heating was obtained, as it is presented in Appendix 1. The knowledge of analytical solution allows to simplify considerably the numerical solution. In particular, in the region of the apex ($x/\tau^{0.5}<<1$) the solution asymptotics can be presented as follows:

$$\theta = \theta_0 + 4(\tau/\pi)^{0.5} - x + \ldots$$

and the temperature gradient in the apex region is constant, $\partial\theta/\partial x=-1$.

Numerical Scheme

The system (3) was numerically integrated, the explicit finite-difference scheme applied. The time derivative was approximated by a first-order forward difference expression, second-order central difference expression was used for the spatial derivative. The discretized equation for the temperature in the node k at the next time step (n+1) reads as

$$\theta_K^{n+1}=(1-2Fo)\,\theta_K^n+Fo[(1+1/k)\,\theta_{K+1}^n+(1-1/k)\,\theta_{K-1}^n]+2dt(1+\exp(\theta_K^n))/k/dx$$

where $Fo=d\tau/dx^2$ - Fourier number. The scheme is stable for Fo <= 0.5. Due to the known asymptotics of the solution in the region of the apex, the singularity of the governing equation (3) at x = 0 is treated easily.

Solution Behaviour and Definition of the Ignition Criterion

Solution behaviour can be described as follows. At the beginning, the temperature inside the substance is not enough to intiate the chemical reaction, and the inert heating due to the external heat flux takes place. After some period of initial heating, when the temperature is high enough for the reaction to occur, both factors of heating are important; and finally, with the further increase of temperature, the chemical heating becomes dominant, and the rapid temperature runaway is observed. The evolution of the temperature distribution with time for the

typical values of the parameters is shown on Fig. 2. In course of the heating process, the apex temperature remains the highest. The dependence of apex temperature on time is shown on Fig. 3.

It is known, that the definition of ignition criterion cannot be done inambiguously, for example, Kulkarny, Kumar and Kuo [1] reviewed 14 definitions of ignition criteria used in studies on ignition of solid propellants. Here the ignition moment is defined as the moment of the most rapid rate of temperature runaway (see Fig. 3), that is, in the absence of depletion, $\tau \to \tau^*$, $\theta(\tau, 0) \to \infty$; and the scale ignition temperature is defined as the apex temperature of inert body at the ignition moment: $\tau=\tau^*$, $\theta_{in}(\tau, 0) = 0$.

Results and Discussion

The results of the calculations can be presented by the following equations:

Ignition criterion, $5<|\theta_0|<25$:

Cone: $$\Omega^* = 0.38 + 0.92|\theta_0|^{-2/3} \quad (4)$$

Ignition criterion for semi-space is given by the equation:

Semi-space: $$\Omega^* = 0.65|\theta_0|^{-2/3} \quad (5)$$

The interpolation equation for the cone ignition criterion versus angle is obtained by comparison of (4) and (5), and within reported accuracy can be written as:

$$\Omega^* = 0.38 \cos\varphi_0 + (0.65+0.26\cos\varphi_0)|\theta_0|^{-2/3} \quad (6)$$

or, in dimensional form:

$$(\rho_g Y)^{\mu} QZ\exp(-E/RT^*)/\, q = 0.38\cos\varphi_0 + (0.65+0.26\cos\varphi_0)(E(T^*-T_0)/RT^{*2})^{-2/3} \quad (6')$$

Thus we have an implicit equation for T^* as a function of angle and other parameters. Equations (2) and (6) together provide the required characteristics of ignition of cone in heterogeneous model. The dependence of ignition temperature on the angle is very weak, and the main factor affecting the temperature is the activation energy. The ignition temperature also logarithmically depends on the external heat flux.

To interpret the results pertaining to the ignition by laser source, one should distinguish between the two possible modes of heating: the first, uniform heating from with the intensity of heat flux q being independent of the angle φ_0, and the second, namely the case of ignition by laser, plane-parallel heating with the intensity of heat flux given by its component, normal to the body surface: $q \sin\varphi_0$. In the latter case, this value

of heat flux should be substituted into the equations (2) and (6), and the ignition delay for the case of ignition by a laser will read as follows:

$$t^*_{2D} = \frac{\pi}{4} \frac{\lambda c \rho \left(T^*(\varphi_0) - T_0\right)^2}{q^2} \frac{\tan^2(0.5\varphi_0)}{\sin^2 \varphi_0} \quad (7)$$

The dependence law of ignition time t* versus angle (2) shows the strong dependence of ignition time upon the angle (proportional to the approximately second power). The ratio of ignition delays by the same intensity heat flux in the two-dimensional and the one- dimensional cases is expressed by the following equation in case of heating by uniform heat flux:

$$\frac{t^*_{2D}}{t^*_{1D}} = \left(\frac{T^*(\varphi_0) - T_0}{T^*(\pi/2) - T_0} \right)^2 \tan^2(0.5\varphi_0) \quad (8a)$$

and by the following equation in case of heating by plane-parallel heat flux:

$$\frac{t^*_{2D}}{t^*_{1D}} = \left(\frac{T^*(\varphi_0) - T_0}{T^*(\pi/2) - T_0} \right)^2 \frac{\tan^2(0.5\varphi_0)}{\sin^2 \varphi_0} \quad (8b)$$

The dependence of the ignition ratios on the angle for the both modes of heating is shown at Fig. 4. For the plane-parallel heating case, the ignition delay for the thin bodies with the apex angle $2\varphi_0$ less than 45° becomes constant, approximately equal to 0.25. One should note, that the ignition delay is reduced four times compared to that for the smooth surface, though the intensity of the heat flux remains the same. On the other hand, if the ignition energy is to be minimized, provided the ignition delay remains the same for the smooth surface and for the rough surface in the shape of the number of the cones, the heat flux or the energy required for the succesful ignition is decreased approximately twice due to the effect of geometry.

CONCLUSIONS

The present research provides an estimation of ignition characteristics of surface irregularities. Analytical solution of the inert problem (without chemical reaction) was obtained. With the use of the temperature averaging procedure multidimensional ignition problem is reduced to effectively one-dimensional, the functional dependence between the ignition paramaters was established. The effect of geometry on ignition was studied. The ignition delays proved to be very sensitive to the apex angle of the body. The law of dependence is approximately quadratic. The energy required for the ignition of the rough surface is at least two times lower than that for the smooth surface, if the other conditions are the same.

APPENDIX 1

Here the analytical solutions of the heat conduction problem referred to in the text are presented.

The solution of system (1') with $\Omega = 0$:

$$\theta = \theta_0 + u^{0.5} g(y/u^{0.5}, \varphi),$$

where

$$g(\xi, \varphi) = \tan^{-1}(0.5\varphi_0) \left[\exp(-0.25\xi^2)/\pi^{0.5} + (0.5\xi+1/\xi)\mathrm{erf}(0.5\xi)\right] - \xi\cos\varphi/\sin\varphi_0 + \xi^{-0.5}\exp(-0.25\xi^2)\sum_{n=1}^{\infty} c_n P_{\mu_n}(\cos\varphi)\int_0^{\infty} z^{2.5}\exp(-z^2) I_{\mu_n+0.5}(z\xi)dz$$

and $c_n = 4\int_{\cos\varphi_0}^{1} zP_{\mu_n}(z)dz \,/\, (\sin\varphi_0 \int_{\cos\varphi_0}^{1} P^2_{\mu_n}(z)dz)$;

$I_n(z)$ - the modified Bessel function of the order of n; $P_m(\cos\varphi)$ - Legendre function of the order of m; erf(z) - error function; and μ_n - the roots of equation:

$P'_m(\cos\varphi_0) = 0$

REFERENCES

1. Kulkarny A.K., Kumar M., Kuo K.K., (1980) "*Review of Solid Propellant Ignition Studies.*", AIAA Paper # 80-1210.
2. Vilyunov V.N., Zarko V.E., (1989) "*Ignition of Solids.*", Elsevier Publishers, Netherlands.
3. Vorsteveld L.G., Hermance C.E., (1987) "Effect of Geometry on Ignition of the Reactive Solid: Square Corner.", *AIAA J.*, v.25, 4, p.592.
4. Vorsteveld L.G., Hermance C.E., (1989) "Effect of Geometry on Ignition of the Reactive Solid: Acute Angles." *J. Propul. Power*, v.5, 1, p.26.
5. Margolin A.D., Mokhin G.N., Krupkin V.G, (1990). "Ignition of Wedge and Cone by Heat Flux in Homogeneous Model of Ignition". Fizika Goreniya I Vzryva, v.26, 1, p.21.

6. Margolin A.D., Mokhin G.N., Krupkin V.G, (1991). "Ignition of Wedge and Cone with Isothermal Foundation by Constant Heat Flux". Fizika Goreniya I Vzryva, v.27, 2, p.3.

7. Margolin A.D., Krupkin V.G, (1991). "Ignition of Wedge and Cone by Variable Heat Flux". Khimicheskaya Fizika, v.10, 8, p.1138.

8. Zeldovich Ya.B., Barenblatt G.I., Librovich V.B., Makhviladze G.M., (1985). " *The Mathematical Theory of Combustion and Explosions.* ", Consultants Bureau, New York and London.

NOMENCLATURE

q - heat flux; Q - heat of reaction; Z - preexponential factor; c - specific heat; ρ - density; λ - thermal conductivity; Y - oxidizer mass fraction; E - activation energy; R - universal gas constant; T - temperature; t - time; r and φ - radial and angular variables of spherical system of coordinates; φ_0 - cone semiangle; T_0 - initial temperature; T* - ignition scale temperature; θ - dimensionless temperature; τ, u - dimensionless time; y, x - dimensionless coordinates; θ_0, Ω, β - dimensionless parameters. Asterisk: * - ignition.

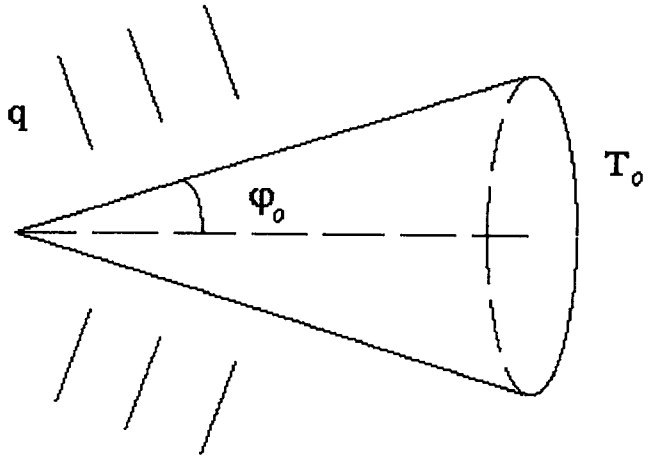

Fig. 1. Model diagram: ignition of cone by constant energy flux.

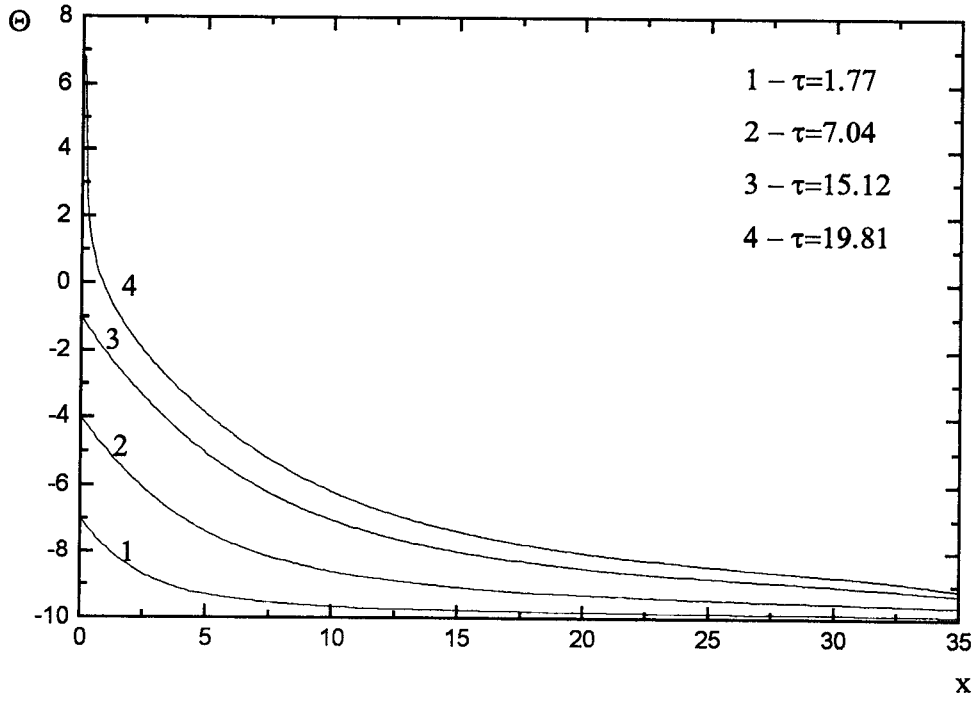

Fig. 2. Temperature distribution inside the cone; $\theta_0 = -10$; $\Omega^* = 0.53$.

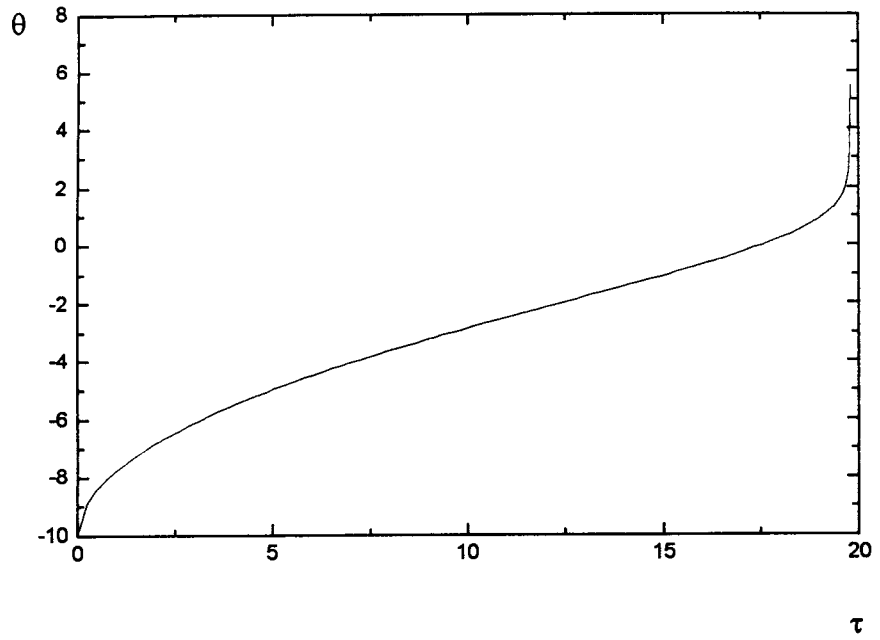

Fig. 3. The dependence of apex temperature upon time; $\theta_0 = -10$; $\Omega^* = 0.53$.

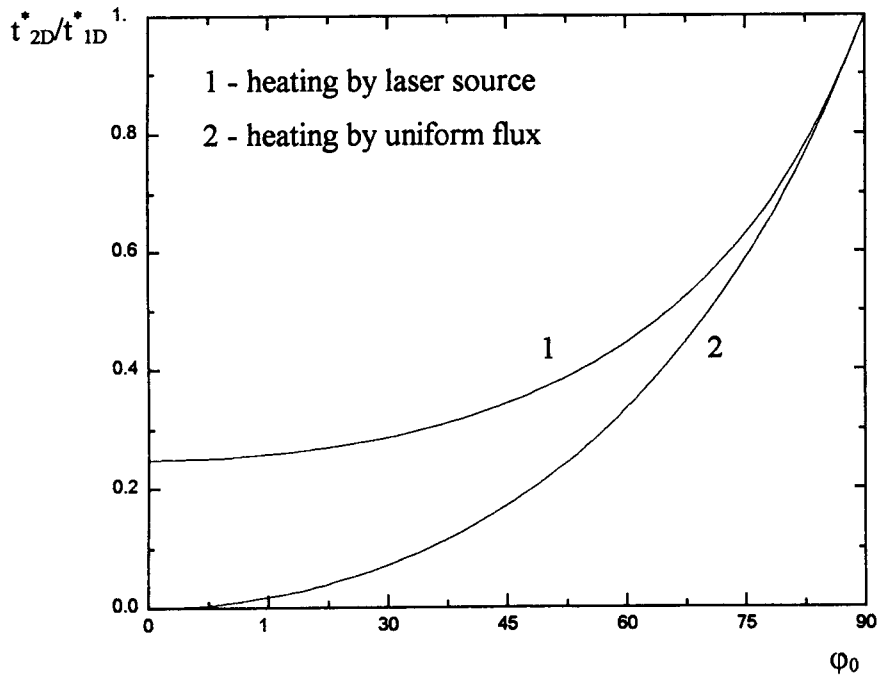

Fig. 4. The ratio of 2-D and 1-D ignition delays vs angle.