UDC 536.46: 533.6

IGNITING A HOMOGENEOUS REACTING MEDIUM BY A HEAT SOURCE WITH FINITE HEAT CONTENT

PMM Vol.40, № 6, 1976, pp.1065-1069
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(Received February 5, 1976)

An asymptotic analysis of the problem of igniting a homogeneous condensed combustible mixture by a flat, cylindrical, or spherical heated body is carried out here with allowance for temperature variation of the body during the process of igniting. An asymptotic solution defining temperature distribution in the region occupied by the condensed medium from the initial instant of time to that of ignition is obtained. The law of temperature variation of the igniting body is determined. A firing criterion that relates basic physicochemical parameters of the problem is derived on the assumption that ignition takes place when during the heat exchange between the igniter and the reacting mixture the igniter is converted from a source to a sink.

The problem of igniting a combustible mixture by an incandescent body is one of the classic problems of the theory of combustion (*). Various aspects of this problem were theoretically investigated in [1 — 3].

1. Statement of the problem. On the usual simplifying assumptions the process of igniting a condensed medium capable of isothermal chemical transformation by an incandescent flat, cylindrical, or spherical body can be defined by the following system of equations:

$$\rho_2 c_2 \frac{\partial T_2}{\partial t_*} = \lambda_2 \frac{1}{r_*^{n-1}} \frac{\partial}{\partial r_*} \left(r_*^{n-1} \frac{\partial T_2}{\partial r_*}\right) + \rho_2 k Q \exp\left(-\frac{E}{RT_2}\right), \qquad r_* \geqslant R_0 \quad (1.1)$$

$$T_2(R_0, t) = T_1(R_0, t), \quad T_2(\infty, t_*) = T_-, \quad T_2(r_*, 0) = T_-$$

$$\frac{\partial T_1}{dt_*} = \frac{\lambda_2 n}{\rho_1 c_1 R_0} \left(\frac{\partial T_2}{\partial r_*}\right)_{r_* = R_0}, \quad T_1 = T_1(t_*), \quad T_1(0) = T_+$$

where t_* is the time, r_* the space coordinate, and R_0 the characteristic dimension of the heated body; $T_1(t)$ is the inert body temperature, $T_2(r_*, t_*)$ is the reacting medium temperature, $n = 1,2,3$ relate to the flat, cylindrical, spherical cases, respectively; λ_i, ρ_i and c_i are the thermal conductivity, density, and specific heat of the inert body $(i = 1)$ and of the condensed phase $(i = 2)$, respectively; k is the preexponential factor, Q is the thermal effect, and T_+° and T_- are initial temperatures of the inert body and of the condensed medium, respectively, with $T_+^\circ > T_-$.

Equation (1.1) defines the heat balance of the inert body. If the thermal diffusivity $\lambda_1 / \rho_1 c_1$ is fairly high, the temperature distribution in the body is uniform, and $T_1(r_*, t_*) = T_1(t_*)$.

*) A. G. Merzhanov and A. E. Averson, Present state of the heat theory of igniting. Moscow, Preprint, Inst. Khim. Fiziki, Akad. Nauk SSSR, 1970. Combustion and Flame, Vol. 16, № 1, 1971.

Problem (1.1) expressed in dimensionless variables is of the form

$$\frac{\partial\theta}{\partial t}=\frac{1}{r^{n-1}}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial\theta}{\partial r}\right)+\delta\exp\frac{\beta(\theta-1)}{\theta+\sigma} \tag{1.2}$$

$$\theta(1,t)=a(t),\quad \theta(\infty,t)=0\ \frac{da}{dt}=\gamma\left(\frac{\partial\theta}{\partial r}\right)_{r=1},\quad a(0)=1$$

$$t_*=R_0^2\rho_2 c_2 t/\lambda_2,\quad r_*=R_0 r,\quad \beta=E/RT_+$$

$$\theta=\frac{T_2-T_-}{T_+-T_-},\quad \sigma=\frac{T_-}{T_+-T_-},\quad a=\frac{T_1-T_-}{T_+-T_-}$$

$$\gamma=\frac{n\rho_2c_2}{\rho_1c_1},\quad \delta=\frac{\rho_2kQR_0^2}{\lambda_2(T_+-T_-)}e^{-\beta}$$

where $a(t)$ and $\theta(r,t)$ are unknown functions that are to be determined in the course of solving the problem, and the assumption of uniform igniter temperature is taken into account.

We shall analyze problem (1.2) on the assumption of high activation energies of the chemical reaction ($\beta\gg 1$), and that parameters γ and σ are of the order of unity. As the instant of ignition we take the instant of time at which the inert body is converted from a heat source to a sink by the initiation of the chemical reaction in the condensed medium. To be able to ignite the inert body must, obviously, have a sufficient heat capacity.

If the igniter heat capacity is low, its temperature drops too quickly and ignition does not take place. On the other hand, when its heat capacity is very high, the temperature decrease and the heat losses up to the instant of ignition are small, and the problem is then virtually the same as that of igniting a condensed phase by an incandescent wall at constant temperature (*). Because of this the solution of the considered problem comprises the estimation of parameter $\delta(\beta)$ which depends on the heat storage capacity of the inert body, as well as the determination of the critical value of δ.

2. Solution. Let us represent the solution of problem (1.2) in the form of the sum

$$\theta=\Phi(r,t)+u(r,t)\,. \tag{2.1}$$

$$\frac{\partial\Phi}{\partial t}=\frac{1}{r^{n-1}}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial\Phi}{\partial r}\right) \tag{2.2}$$

$$\Phi(1,t)=a(t),\quad \Phi(\infty,t)=0,\quad \Phi(r,0)=0$$

Using the Laplace transformation we obtain

$$\Phi^*(r,p)=\begin{cases}\dfrac{a_*(p)}{r}e^{-\sqrt{p}(r-1)}\\ a^*p=\dfrac{K_0(r\sqrt{p})}{K_0(\sqrt{p})},\\ a^*(p)e^{-\sqrt{p}(r-1)}\end{cases}\quad \left(\frac{\partial\Phi^*}{\partial r}\right)_{r=1}=\begin{cases}-a^*(\sqrt{p}+1), & n=3\\ a^*\sqrt{p}\dfrac{K_1(\sqrt{p})}{K_0(\sqrt{p})}, & n=2\\ -a^*\sqrt{p}, & n=1\end{cases}$$

$$\Phi^*(r,p)=p\int_0^\infty e^{-pt}\Phi(r,t)\,dt$$

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*) V. S. Berman, Certain problems of the theory of spreading of the zone with isothermal and chemical reactions in gaseous and condensed media. Candidates dissertation, Moscow, 1974, Inst. Problem Mekhaniki, Akad. Nauk SSSR.

where K_0 and K_1 are Macdonald functions of order zero and unity, respectively.

In conformity with (2.1) for $u\ (r,\ t)$ from (1.2), we obtain

$$\frac{\partial u}{\partial t}=\frac{1}{r^{n-1}}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial u}{\partial r}\right)+\delta(\beta)\exp\left[\beta\left(\frac{\Phi+u-1}{\Phi+u+\sigma}\right)\right] \tag{2.3}$$

$$u(1,t)=u(\infty,t)=u(r,0)=0$$

$$\frac{da}{dt}=\gamma\left[\left(\frac{\partial\Phi}{\partial r}\right)_{r=1}+\left(\frac{\partial u}{\partial r}\right)_{r=1}\right],\quad a(0)=1$$

To analyze the problem we separate in the region $1\leqslant r<\infty$ the boundary layer at the surface of the inert body, and introduce in that layer the variables $x=(r-1)\psi(\beta)$, where $\psi(\beta)\gg 1$.

In the dimensionless variables used here the time of ignition is considerably smaller than unity, hence we can substitute the new variable $\tau=t\varphi(\beta)$ and $\varphi(\beta)\gg 1$.

We seek a solution of the form

$$a(t)=1+\beta^{-1}a_1(\tau)+\ldots,\quad u(x,t)=\beta^{-1}u_1+\ldots$$

Analysis shows that the solution which corresponds to ignition is that when $\psi^2=\varphi\beta^2$, $\psi=\beta^2$, $\varphi=\beta^2$, $\delta=\delta_0\beta^{\circ}$, $\delta_0=O(1)$. Substituting $a(t)$ and $u(x,t)$ into (2.3) we obtain

$$\frac{\partial^2 u_1}{\partial x^2}+\delta_0\exp\frac{a_1+u_1-x/\sqrt{\pi t}}{1+\sigma}=0 \tag{2.4}$$

$$u_1(0,\tau)=0,\quad u_1(x,0)=0,\quad u_1(\infty,\tau)=O(1)$$

$$\frac{da_1}{d\tau}=\gamma\left[-\frac{1}{\sqrt{\pi\tau}}+\left(\frac{\partial u_1}{\partial x}\right)_{x=0}\right],\quad a_1(0)=0 \tag{2.5}$$

The general solution of Eq. (2.4) is of the form

$$u_1(x,\tau)=\frac{x}{\sqrt{\pi\tau}}-a_1(\tau)+ \tag{2.6}$$

$$(1+\sigma)\left[-\ln\delta_0+\ln c_2(\tau)-2\ln\operatorname{ch}\left(c_1(\tau)+x\sqrt{\frac{c_2(\tau)}{2(1+\sigma)}}\right)\right]$$

By satisfying boundary conditions at $x=0$ and $x=\infty$ we obtain

$$\operatorname{ch}^2 c_1(\tau)=\delta_0^{-1}\exp\left(-\frac{a_1(\tau)}{1+\sigma}\right)c_2(\tau),\quad c_2(\tau)=\frac{1}{2\pi(1+\sigma)\tau}$$

The temperature gradient at the igniter surface $r=1$ $(x=0)$ is

$$\left(\frac{\partial\theta}{\partial r}\right)_{r=1}=-(\pi r)^{-1/2}\left[1-2\pi(1+\sigma)\delta_0\tau\exp\frac{a_1}{1+\sigma}\right]^{1/2} \tag{2.7}$$

This shows that the heat flux vanishes when the expression in brackets is zero. At that instant the inert body changes from a heat source to a sink (the instant of ignition).

With allowance for (2.7) from (2.5) we obtain

$$\frac{ad_1}{d\tau}=-\gamma(\pi\tau)^{-1/2}\left[1-2\pi(1+\sigma)\delta_0\tau\exp\frac{a_1}{1+\sigma}\right]^{1/2},\quad a_1(0)=0 \tag{2.8}$$

Passing to new variables, instead of (2.8) we obtain

$$dy/d\xi=\varepsilon\sqrt{1-\xi^2e^{-y}},\quad y(0)=0,\quad y\geqslant 0 \tag{2.9}$$

$$a_1=-y(1+\sigma),\quad \tau=\frac{\xi^2}{2\pi(1+\sigma)\delta_0},\quad \varepsilon=\frac{\gamma}{\pi}\sqrt{\frac{2}{(1+\sigma)^3\delta_0}}$$

The form of solution (2.9) depends on parameter ε. If ε is fairly great, it exists in the whole of the interval $0 \leqslant \xi \leqslant \infty$, while for fairly small ε it obtains only in a finite interval of time variation, which corresponds to ignition. The critical value $\varepsilon = \varepsilon^*$, determined by numerical integration, is $\varepsilon^* = 1.138$. It follows from this that ignition takes place when $R_0 \geqslant R_0^*$, while for $R_0 < R_0^*$ ignition does not occur and

$$R_0^* = 0.395 \frac{n\rho_2 c_2}{\rho_1 c_1} \left(\frac{E}{RT_+}\right)^{3/2} \left(\frac{T_+ - T_-}{T_+}\right)^{3/2} \left[\frac{\lambda_2 (T_+ - T_-)}{\rho_2 KQ}\right]^{1/2} \exp \frac{E}{2RT_+} \qquad (2.10)$$

It is obvious that the indicated criterion is valid in the case of asymptotic behavior of solution in which the inert body temperature variation during ignition is substantial, as well as that in which this variation is negligible.

The obtained formulas determine the temperature distribution in the inner zone, the igniter temperature variation, and the critical conditions of ignition. For defining temperature variation throughout the condensed medium zone $R_0 < r < \infty$ these formulas must be supplemented by the temperature distribution in the outer zone $u = \beta^{-1} U_1$, where function U_1 is the solution of the following linear problem:

$$\partial U_1 / \partial \tau = \partial^2 U_1 / \partial X^2, \quad X = (r - 1)\beta$$

$$U_1(0, \tau) = u_1(x \to \infty, \tau) = f(\tau), \quad U_1(X, 0) = U(\infty, \tau) = 0$$

$$U_1(X, \tau) = \frac{X}{2\sqrt{\pi}} \int_0^{\pi} \frac{f(\tau')}{(\tau - \tau')^{3/2}} \exp\left[-\frac{X^2}{4(\tau - \tau')}\right] d\tau'$$

As an example, let us consider igniting nitromethane by a flat copper rod. In this case the phisico-chemical properties are as follows [4]:

$$\rho_1 = 8.939 \text{g}\cdot\text{cm}^{-3}; \quad c_1 = 9.154\cdot 10^{-2} \text{ cal}\cdot\text{g}^{-1}\cdot{}^\circ\text{K}^{-1}; \quad \rho_2 = 1.1286 \text{ g}\cdot\text{cm}^{-3};$$

$$c_2 = 4.153\cdot 10^{-1} \text{ cal}\cdot\text{g}\cdot{}^\circ\text{K}^{-2}; \quad \lambda_1 = 5\cdot 10^{-4} \text{ cal}\cdot\text{cm}^{-1}\cdot\text{sec}^{-1}\cdot{}^\circ\text{K}^{-1};$$

$$Q = 1.113\cdot 10^{-3} \text{ cal}\cdot\text{g}^{-1}; \quad k = 3.98\cdot 10^{-14} \text{ sec}^{-1}; \quad E = 5.36\cdot 10^4 \text{ cal}\cdot\text{mole}^{-1}\cdot{}^\circ\text{K}^{-1}.$$

The initial temperature of nitromethane is $T_- = 300°$ K. The dependence of the critical dimension of the igniter (half-width of rod) on the initial temperature T_+ is shown in Fig. 1. The region above the curve corresponds to ignition. The critical dimension of a cylindrical or spherical igniter can be obtained from Fig. 1 by simple calculation.

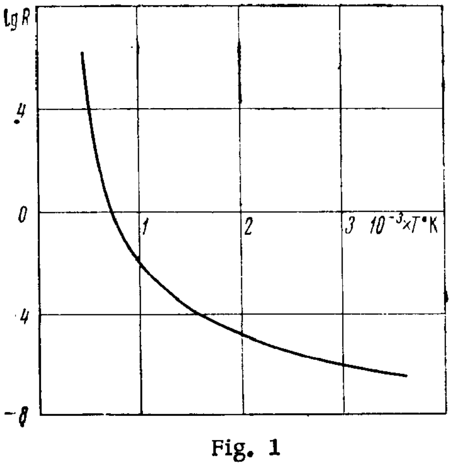

Fig. 1

Note that in the considered case the solution of the problem implies that the dimensions of the zone with chemical heat release are considerably smaller than the dimensions of the igniter so that the problem in the inner zone is plane, and the igniter shape manifests itself only by the presence in formulas of the factor n which is equal to the ratio of the igniter area to its volume.

The above analysis is based on the assumption that $\gamma = O(1)$, which corresponds to typical values of thermophysical properties of the igniter and condensed medium. A similar analysis may be carried out on a more general assumption as regards parameter γ. If $\gamma = \gamma_0 \alpha(\beta)$ with $\gamma_0 = O(1)$, the igniter temperature variation is substantial for $\sigma(\beta)\alpha^{-2}(\beta)\beta^{-3} = O(1)$. In that case the variables in the inner zone are to be of the form $x = (r-1)\alpha\beta^2$ and $\tau = t\alpha^2\beta^2$, and for α satisfying the inequality $\alpha\beta^2 \gg 1$, the solution is determined by the derived here formulas in which $\delta / \alpha^2\beta^3$ and γ / α are to be substituted for δ_0 and γ, respectively. If, however, $\alpha = \beta^{-2}$ the problem reduces to the solution of an equation in which the differential operator retains the form determined by the problem symmetry.

We note in conclusion that the problem of igniting a reacting gas by a heated body with allowance for the cooling of the igniter and the burnout of reagent can be treated by the method developed here. In that case the problem reduces to the integration of two nonlinear integral equations for the igniter temperature and concentration of reagent at its surface.

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Translated by J. J. D.

UDC 539.3

THE REPRESENTATION OF THE DISPLACEMENT GRADIENT OF ISOTROPIC ELASTIC BODY IN TERMS OF THE PIOLA STRESS TENSOR

PMM Vol. 40, № 6, 1976, pp. 1070-1077

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(Received May 28, 1976)

The representation of the displacement gradient of an isotropic elastic body is analyzed. It is shown on the basis of a single controlling inequality and a polar expansion of the Piola tensor that such representation has generally four branches. The mechanical meaning and the nature of that ambiguity is explained. It is established that when the angles of turn of material fibers are not excessively large, only one of the four branches is obtained. Particular cases in which the nature of ambiguity is more complex are investigated. It is noted that in many practical problems the representation of the displacement gradient by the Piola stress tensor is unambiguous.