PMM U.S.S.R., Vol.44, pp.60-64
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0021-8928/81/1 0060 $7.50/0
UDC 536.46:533.6+534.222.2

ASYMPTOTIC ANALYSIS OF THE PROCESS OF IGNITING A COMBUSTIBLE GAS MIXTURE BY THERMAL INHOMOGENEITY *

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An approximate solution is obtained for the problem of igniting a gaseous combustible mixture in which a region of higher temperature is created at the initial instant of time. The temperature in the heated region either sharply increases or decreases with time depending on the properties of the active gaseous mixture and on the initial temperature distribution. An initial small temperature increase followed by its decrease is also possible. In the first case ignition take place, while in the second the initial temperature inhomogeneity becomes blurred in time. Approximate equations defining the initial stage of the process are derived, and critical values of characteristic parameters corresponding to ignition are established.

The analysis is based on the use of the dimensionless ratio of the maximum temperature in the heated zone to the activation temperature, as the small parameter commonly used in the theory of combustion. We consider the case of plane geometry in which the heated region is one-dimensional and symmetric about the maximum initial temperature plane in which we locate the coordinate origin. The method developed here enables us to extend the obtained results to cases of cylindrical and spherical geometries.

The use of asymptotic methods in the theory of ignition makes it often possible to reduce a complex nonlinear problem to the analysis of simpler approximate equations which in particular cases can be solved analytically, and to indicate dimensionless parameters that define the basic particulars of the process /1—7/. An asymptotic analysis of the problem of igniting a reacting medium by a light flux is presented in /1,2/, and asymptotic solutions of the problem of igniting a reacting medium by a heated body at constant or varying temperature appear in /3—6/. In all of these problems the igniting source was assumed to act at the reacting medium boundary.

1. Statement of the problem.

On the basis of the usual assumptions of the theory of combustion /8/ the single-stage exothermic chemical reaction in gas can be defined by the following system of equations:

$$\begin{gathered}\rho c\frac{\partial T}{\partial t'}=\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)-mc\frac{\partial T}{\partial z}+\\ Qk\rho^n(1-y)^n\exp\left(-\frac{E}{RT}\right)-\alpha'(T-T_-)\\ \rho\frac{\partial y}{\partial t'}=\frac{\partial}{\partial z}\left(D\rho\frac{\partial y}{\partial z}\right)-m\frac{\partial y}{\partial z}+k\rho^n(1-y)^n\exp\left(-\frac{E}{RT}\right)\\ \frac{\partial\rho}{\partial t'}+\frac{\partial m}{\partial z}=0,\quad T\rho=\mathrm{const}\end{gathered}\tag{1.1}$$

where T is the temperature, y is the concentration of reaction products, $\rho=\rho(T)$ is the density, $\lambda=\lambda(T)$ is the thermal conductivity, c is the specific heat, z is a space coordinate, t' is the time, Q is the thermal yield of the reaction, k is the frequency factor, E is the activation energy, n is the reaction order, R is the gas constant, $D=D(T)$ is the diffusion coefficient, m is the mass velocity of gas, T_- is the temperature at considerable distance from the heated region, α' is the heat transfer coefficient, and T_0 is the maximum temperature in the heated region at the initial instant of time. The possibility of heat removal from the combustion zero, which occurs when the gas is contained in a fairly thin plane layer between two heat conducting surfaces, is taken into account in Eqs. (1.1). When $\alpha'=0$ there is obviously no heat transfer.

We assume that at the initial instant of time the temperature distribution in the gas is defined by formula

$$\begin{gathered}T(z,0)=(T_0-T_-)\Phi(z/l_T)+T_-\\ d\Phi(0)/dz=0,\quad d^2\Phi/dz^2<0,\quad\Phi(0)=1,\quad\Phi(\pm\infty)=0\end{gathered}\tag{1.2}$$

where l_T is the characteristic scale of the initial temperature distribution variation. We pass from variables (t',z) to variables (t',ψ) using formulas

$$m=-\partial\psi/\partial t',\quad\rho=\partial\psi/\partial z,\quad m(z,0)=0,\quad\psi(z=0,t')=0$$

and assume that

$$\lambda\rho=\mathrm{const},\quad c=\mathrm{const},\quad D\rho^2=\mathrm{const}$$

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*Prikl.Matem.Mekhan.,44,No.1,89-95,1980

We write the equations, boundary and initial conditions in dimensionless variables in the form

$$\frac{\partial\Theta}{\partial t}=\frac{\partial^2\Theta}{\partial X^2}+\delta(1-y)^n\Gamma(\Theta)\exp(\beta(\Theta-1))-\alpha\Theta \tag{1.3}$$

$$\frac{\partial y}{\partial t}=L^{-1}\frac{\partial^2 y}{\partial X^2}+\delta\gamma(1-y)^n\Gamma(\Theta)\exp(\beta(\Theta-1))$$

$$\Theta(X,0)=\Phi(X),\quad y(X,0)=0$$

$$X=\frac{\psi}{\Delta x},\quad t=\frac{t'}{\Delta t},\quad \Delta x=l_{\text{т}}\rho$$

$$\beta^{-1}=\frac{RT_0^2}{E(T_0-T_-)},\quad \gamma=\frac{c(T_0-T_-)}{Q},\quad L=\frac{\lambda}{D\rho c}$$

$$\rho_0=\rho_0(T),\quad \Theta=\frac{T-T_-}{T_0-T_-},\quad \Gamma(\Theta)=\left(\frac{\rho}{\rho_0}\right)^{n-1}$$

$$\alpha=\frac{\tau_{\text{т}}}{\tau_\alpha},\quad \delta=\frac{\tau_{\text{т}}}{\gamma\tau_{ch}},\quad \Delta t=\frac{cl_{\text{т}}^2\rho_0}{\lambda}$$

$$\tau_{\text{т}}=\frac{l_{\text{т}}^2\rho_0 c}{\lambda},\quad \tau_{ch}=\frac{\exp(E/RT_0)}{k\rho_0^{n-1}},\quad \tau_\alpha=\frac{\alpha'}{\rho c}$$

where τ_T is the characteristic time of relaxation due to heat conduction, τ_{ch} is the characteristic time of the chemical reaction, τ_α is the characteristic time of thermal relaxation related to the "lateral" heat transfer, and γ^{-1} is the ratio of the specific chemical heat value to the initial heating heat content at the point of maximum temperature.

The basic aim of the approximate asymptotic solution of problem (1.3) is the determination of the critical value of δ which separates two modes by investigating the initial stage of the process. When $\delta > \delta^*$ ignition takes place, while for $0 < \delta < \delta^*$ we have extinction. We shall derive a solution for $\beta \gg 1$ typical for the majority of gases producing exothermic reactions. Unless otherwise stated, we assume that

$$L,\ n,\ \Gamma,\ \alpha,\ \gamma,\quad \partial F/\partial\Theta=O(1)$$

2. Solution of the problem.

We seek a solution of the form

$$\Theta(X,t)=\Theta_i(X,t)+U(X,t,\beta) \tag{2.1}$$

where Θ_i is the solution of the problem which defines the heating of gas as that of a chemically inert body

$$\partial\Theta_i/\partial t=\partial^2\Theta_i/\partial X^2-\alpha\Theta_i \tag{2.2}$$

$$\Theta_i(X,0)=\Phi(X),\quad \Phi(0)=1,\quad d\Phi(0)/dX=0$$

$$d^2\Phi/dX^2<0$$

whose solution is of the form

$$\Theta_i(X,t)=\frac{e^{-\alpha t}}{2\sqrt{\pi t}}\int_{-\infty}^{\infty}\Phi(\eta)\exp\left(-\frac{(X-\eta)^2}{4t}\right)d\eta \tag{2.3}$$

$$\Theta_i(0,0)=1$$

The most favorable conditions for ignition are, obviously, near the point of the highest initial temperature. The temperature at that point varies in conformity with the law

$$\Theta_i(0,t)=\frac{e^{-\alpha t}}{2\sqrt{\pi t}}\int_{-\infty}^{\infty}\Phi(\eta)\exp\left(-\frac{\eta^2}{4t}\right)d\eta,\quad \Theta_i(0,0)=1 \tag{2.4}$$

Note that when the heat energy balance determined by the relation between heat dissipation and its generation by the chemical reaction in the neighborhood of point $X=0$ becomes negative at instants of time close the initial, ignition becomes impossible.

Thus for the determination of critical conditions of ignition it is sufficient to analyze the evolution of the temperature initial perturbation in the close vicinity of the maximum temperature point. It follows from (2.3) that the temperature distribution during the short time of passive heating-up near that point is defined by

$$\Theta_i(X,t)=1+\frac{d^2\Phi(0)}{dX^2}\left[\frac{X^2}{2}+t\right]-\alpha t+O(X^2,t) \tag{2.5}$$

For analyzing temperature variation due to chemical heating-up we separate the region of variation of variables X and t in which the chemical heating-up is substantial (the inner region) and the region where the chemical heating-up can be neglected (the external region).

We introduce in the inner region new variables $\tau=t\beta$ and $\xi=X\sqrt{\beta}$, and seek for U and y a solution of the form

$$U(X,t,\beta)=\beta^{-1}U_1(\xi,\tau)+\beta^{-2}U_2(\xi,\tau)+O(\beta^{-3}) \tag{2.6}$$

$$y(X,t,\beta)=y_0(\xi,\tau)+\beta^{-1}y_1(\xi,\tau)+O(\beta^{-2})$$

We assume that

$$\delta = f_0(\beta)\,\delta_0 + f_1(\beta)\,\delta_1, \quad \lim_{\beta\to\infty} \frac{f_1(\beta)}{f_0(\beta)} \to 0 \tag{2.7}$$

Formula (2.7) implies that generally the order of δ relative to β can vary. Substituting (2.6) and (2.7) into (1.3) and taking into account (2.5), for the principal terms of expansion (2.6) we obtain

$$\frac{\partial U_1}{\partial \tau} = \frac{\partial^2 U_1}{\partial \xi^2} + f_0\delta_0(1-y_0)^n\Gamma\exp\left[U_1 - \alpha\tau + \frac{d^2\Phi(0)}{dX^2}\left(\frac{\xi^2}{2}+\tau\right)\right] \tag{2.8}$$

$$\frac{\partial y_0}{\partial \tau} = \frac{\partial^2 y_0}{\partial \xi^2} + \beta^{-1}\gamma f_0\delta_0\Gamma(1-y_0)^n\exp\left[U_1 - \alpha\tau + \frac{d^2\Phi(0)}{dX^2}\left(\frac{\xi^2}{2}+\tau\right)\right] \tag{2.9}$$

$$U_1(\xi,\ 0) = 0, \quad y_0(\xi,\ 0) = 0 \tag{2.10}$$

$$\frac{\partial U_1(0,\ \tau)}{\partial \xi} = 0, \quad \frac{\partial y_0(0,\ \tau)}{\partial \xi} = 0$$

It follows from (2.8) that for δ close to δ^* the second term in the right-hand side of the equation must be of the same order in β^{-1} as the others, i.e. $f_0(\beta) = 1$. Then from (2.9) and (2.10) we have $y_0 \equiv 0$.

Thus in the initial stage of the process the temperature rise of chemical heating-up is substantial for a negligibly small burn-up of the reagent. Depending on δ_0 Eq. (2.8) must determine different types of behavior of function $U_1(\tau, \xi)$: a monotonically increasing one corresponding to ignition, the other nonmonotonic has a section of growth followed by a drop that corresponds to extinction. The conditions of merging of the internal solution with the external is automatically satisfied as $\xi \to \infty$, hence there is no necessity to examine these. The determination of δ^* generally requires the numerical solution of problem (2.8).

3. Particular cases.

Let us consider particular cases taking into account that $y_0 \equiv 0$. We represent Eq. (2.8) as

$$\frac{\partial U_1}{\partial \tau} = \frac{\partial^2 U_1}{\partial \xi^2} + \delta_0\exp\left[U_1 - \alpha\tau + \Phi''(0)\left(\frac{\xi^2}{2}+\tau\right)\right] \tag{3.1}$$

$$U_1(\xi,\ 0) = 0, \quad U_{1\xi}(0,\ \tau) = 0, \quad U_1(\infty,\ \tau) = 0$$

and consider the case when $\alpha \neq 0$ and $d^2\Phi(0)/dX^2 = 0$, i.e. when functions Φ with $X \to 0$ are of the form $\Phi = 1 - O(X^n)$, where $n \neq 2$.

Since the initial conditions are independent of ξ when $\tau > 0$, we have

$$U_1(\xi,\ \tau) = U_1(\tau), \quad \partial U_1/\partial\tau = \delta_0\exp(U_1 - \alpha\tau), \quad U_1(0) = 0 \tag{3.2}$$

from which

$$U_1 = -\ln\left[1 - \delta/\alpha + \delta/\alpha e^{-\alpha\tau}\right] \tag{3.3}$$

Solution (3.3) depends on the quantity δ/α: for $0 < \delta/\alpha < 1$ it increases from $U_1(0)$ to its maximum value

$$U_1(\infty) = -\ln\left[1 - \delta/\alpha\right] > 0$$

as $t \to \infty$.

When $\delta/\alpha = 1$ the solution is of the form $U_1 = \alpha\tau$, and as $\tau \to \infty$ it approaches infinity. For $\delta/\alpha > 1$ the solution is of the explosion type, and for $\bar{\tau} = -{}^1\!/_2\ln(1 - \alpha/\delta)$ the temperature $U_1(\bar{\tau}) = \infty$. Hence $\delta^* = \alpha$. In dimensional form

$$\frac{\delta}{\alpha} = \frac{kQ\rho_0^{n-1}\exp(-E/RT_0)}{\alpha'(T_0 - T_-)}$$

i.e. in the case of $\Phi''(0) = d^2\Phi(0)/dX^2 = 0$ with $\alpha \neq 0$ and $\delta/\alpha > 1$ ignition takes place, and for $\delta/\alpha < 1$ extinction. It should be pointed out that in this case the initial size of the elevated temperature zone is immaterial.

In order to reduce the number of independent parameters it is convenient to introduce in the case of $\Phi''(0) \neq 0$ new parameters

$$\eta = \xi(|\Phi''(0)|)^{1/2}, \quad p = \tau|\Phi''(0)|$$

$$b = \delta_0|\Phi''(0)|^{-1}, \quad a = \alpha|\Phi''(0)|^{-1}$$

with which Eq. (3.1) assumes the form

$$\partial U_1/\partial p = \partial^2 U_1/\partial\eta^2 + b\exp(U_1 - (a+1)p - \eta^2/2) \tag{3.4}$$

$$U_1(\eta, p = 0) = 0, \quad U_{1\eta}(0, p) = 0, \quad U_1(\infty, p) = 0$$

Because of the presence of the term $-\eta^2/2$ in the exponent in (3.4) which implies a rapid decrease of the heat emission function, it is possible to consider in the approximate analysis instead of (3.4) the equation

$$\partial v/\partial p = b_0\exp(v - (a+1)p), \quad v(p = 0) = 0 \tag{3.5}$$

Note that the critical value $b_0{}^*$ which corresponds to Eq. (3.5) is lower than b^* which corresponds to Eq. (3.4). This is due to the presence in (3.4) of the diffusion term $\partial^2 U_1 / \partial\eta^2$ which represent heat transfer from the zone of increased temperature. The approximate equation (3.5) yields however a correct qualitative picture of the process.

From (3.5) we obtain

$$v = -\ln\left[(b_0 / (a+1))\left(e^{-(a+1)p} - 1\right) + 1\right] \qquad (3.6)$$

which yields the critical value of $b_0{}^*$ as $b_0{}^* = a + 1$, the cases of $b_0 < a + 1$ and $b_0 > a + 1$ correspond, respectively, to extinction and ignition. In dimensional form the condition of ignition is

$$\frac{kQ\rho_0^{n-1}\exp(-E / RT_0)}{(T_0 - T_-)(\alpha' + \Phi''\lambda\rho_0 l_T^{-2})} \gg 1$$

The curve of $b_0{}^* = b_0{}^*(a)$ is shown in Fig.1 by the dash line.

Equation (3.4) was also solved numerically for the initial temperature distribution $\Phi(X) = \exp(-X^2 / 2)$. It is represented in Fig.1 in the form of function $b(a)$. The values of parameters in the region above that curve correspond to ignition, those below it to extinction. Calculations had shown that in the absence of heat transfer $a = 0$ the critical value is $b^* = 1.7$, while the critical value calculated by formula (3.6) yields $b_0{}^* = 1$. This shows that even a rough investigation provides correct qualitative conclusions.

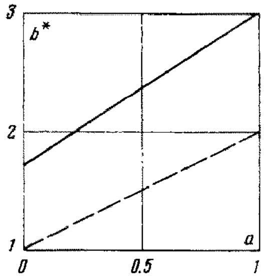

Fig.1

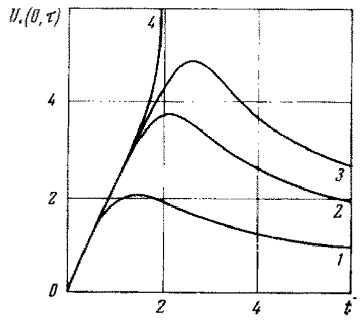

Fig.2

Curves 1—4 in Fig.2 show the dependence of chemical heating-up maximum temperature $U_1(0, \tau)$ on time for fixed $b = 2.5$ and $a = 0.8$, 0.65, 0.675, 0.6. The qualitative change of the shape of curves occurs for $a = 0.6$.

To check the exactness of asymptotic methods, the complete problem (1.3) was solved numerically for $\Phi = \exp(-X^2/2)$ and $\alpha = 0$. The results of calculations are shown in Fig.3. The complete temperature field pattern appears in Fig.3a, where the heavy solid line is the characteristic of the initial high temperature cone. The solid lines 1 and 2 show the temperature variation with time in the case of ignition for $\delta = 1.55$, $\beta = 10$, and $t_1 < t_2$. The dash lines define the space-time temperature distribution in the case of extinction for $\delta = 1.21$ and $\beta = 10$ at the same instants of time $t_1 < t_2$.

The dependence of δ^* on β is shown in Fig.3,b; ignition occurs for parameters lying above the curve. Since the precision of asymptotic methods increases as $\beta \to \infty$, it is reasonable to compare the asymptotic and numerical solutions for $\beta \to \infty$. For $\alpha = 0$ from the approximate problem (3.1) we have $b^* = 1.7$. Computations by (1.3) and Fig. 3,b show that for $\alpha = 0$ and $\beta = 50$, we have $\delta^* = 1{,}71$, i.e. a good agreement of results. Although Eq. (3.1) is not always solvable analytically, it makes possible the examination of interesting particular cases that correspond to various $d^2\Phi / dX^2$ and α, and to obtain qualitative characteristics of a process.

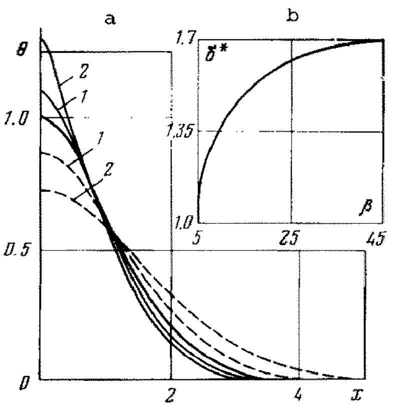

Fig.3

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Translated by J.J.D.