ON THE THEORY OF FLAME PROPAGATION

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The following scheme [1] is considered in studying flame propagation. There is an infinite rod in which the combustion process is initiated. The temperature distribution in the rod is described by Equation

$$\frac{\partial T}{\partial t} = a^2 \frac{\partial^2 T}{\partial x^2} + F(T)$$

with an initial temperature distribution of the form shown in Fig.1. The function $F(T)$ characterizing the heat release during the combustion process has the form shown in Fig.2. A solution of the form $T(x - \omega t)$, i.e. a solution in the form of waves traveling with velocity ω , is sought. It is

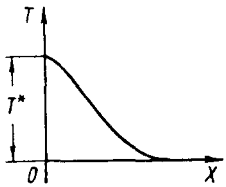

Fig. 1

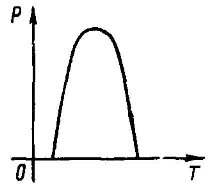

Fig. 2

proved that there exists a solution of the mentioned form, which is unique, corresponding to the value of ω which characterizes the flame propagation velocity. A problem of analogous kind is considered in [2], but it is assumed that

$$F(0) = F(T^*) = 0, \quad F'(0) = \beta, \quad F'(T) \leqslant \beta, \quad T \geqslant 0$$

It is shown that the value of ω may be evaluated by means of Formula

$$\omega = 2a\sqrt{\beta}$$

However, it is known that many exothermal processes are characterized by functions $F(T)$ for which the condition $F'(0) \geqslant F'(T)$ is not satisfied. In particular, explosive processes are characterized by functions $F(T)$ which grow slowly for small T and very rapidly at high temperatures [3].

For these processes a slow development in the initial period (the period of induction) and a very rapid development after the attainment of a definite temperature (period of explosion) is characteristic. It is also known [3] that the diameter of the vessel has essential influence on the rapidity of the process. It is natural to assume that the effect of the factors mentioned should be analogous in flame propagation processes and an attempt has been made, along these lines, to find an explanation of the process of the rapid growth of the flame velocity during the transition from combustion into detonation, and also of the influence of the vessel diameter on the propagation velocity. However, a direct examination of the nonlinear problem is difficult (especially in a two-dimensional model). Hence, first the linear one-dimensional model of flame propagation without taking account of combustion of the material is considered herein.

It turns out that neglecting the combustion does not affect the limiting flame velocity. The obtained result is used to analyze nonlinear effects.

However, the one-dimensional theory can not explain the influence of the vessel diameter on the propagation velocity. A theory taking account of the radial change in temperature is considered in the second part, and this permits the introduction of the concept of critical vessel diameter and the obtaining of a dependence of the propagation velocity on the coefficient of thermal diffusivity.

1. Let us consider a semi-bounded pipe in which there is a combustible substance at the temperature $T = 0$. A temperature $T = T_0$ is applied to the end $x = 0$ at a certain instant. Then, considering the temperature to be constant at each cross section (one-dimensional theory), we have (assuming $F(T) = \beta T$)

$$\frac{\partial T}{\partial t} = a^2 \frac{\partial^2 T}{\partial x^2} + \beta T, \qquad T \mid_{t=0} = 0, \qquad T \mid_{x=0} = T_0 \tag{1.1}$$

Henceforth it is convenient to consider the case when $T|_{x=0} = T_0$ for $0 < t < t_0$, $T|_{x=0} = 0 \ (t > t_0)$ Evidently this case is closer to the real process of initiation of combustion.

Let us put $T = ue^{\beta t}$, then

$$\frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial x^2}, \qquad u \mid_{t=0} = 0, \qquad u \mid_{x=0} = T_0 e^{-\beta t}$$

The solution of this problem is written as [4]

$$u(x, t) = \frac{xT_0}{2a\sqrt{\pi}} \int_0^t \frac{e^{\beta t}}{\sqrt{(t-\tau)^3}} \exp \frac{-x^2}{4a^2(t-\tau)} \, d\tau$$

and hence

$$T(x, t) = \frac{xT_0}{2a\sqrt{\pi}} \int_0^t \frac{e^{\beta(t-\tau)}}{\sqrt{(t-\tau)^3}} \exp \frac{-x^2}{4a^2(t-\tau)} \, d\tau \tag{1.2}$$

Under the assumptions that $T|_{x=0} = T_0 \ (0 < t < t_0)$, $T|_{x=0} = 0 \ (t > t_0)$, we have from (1.2) for $t > t_0$

$$T(x, t) = \frac{xT_0}{2a\sqrt{\pi}} \int_0^{t_0} \frac{e^{\beta(t-\tau)}}{\sqrt{(t-\tau)^3}} \exp \frac{-x^2}{4a^2(t-\tau)} \, d\tau$$

Considering t large and t_0 small, we may put $t - \tau = t$ and

$$T(x, t) \approx \frac{xT_0 t_0}{2a\sqrt{\pi}} \frac{e^{\beta t}}{\sqrt{t^3}} \exp \frac{-x^2}{4a^2 t} \tag{1.3}$$

Let us interpret the flame propagation as the advancement of a certain constant temperature. Then we obtain a relationship connecting x and t

$$\frac{x t_0 T_0}{2a\sqrt{\pi}} \frac{e^{\beta t}}{\sqrt{t^3}} \exp \frac{-x^2}{4a^2 t} = \text{const}$$

It is easy to see that this equation has an asymptotic solution of the form

$$x = 2a\sqrt{\beta}t - A \ln t + B \qquad (A,\ B = \text{const})$$

as $t \to \infty$.

Hence, for

$$dx\ /\ dt = 2a\sqrt{\beta} \quad \text{for} \quad t \to \infty$$

that is, for the limiting flame propagation velocity, the same value has been obtained as in [2]. Ttherefore, taking account of the combustion has no effect on the limiting flame propagation velocity. This fact is easily explained physically. Heat from distantly removed points does not affect the propagation velocity, only the coefficient β and the heat transfer to nearby points are of fundamental importance

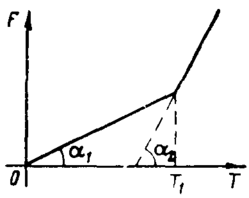

Fig. 3

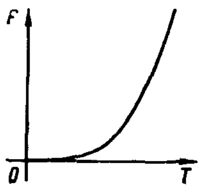

Fig. 4

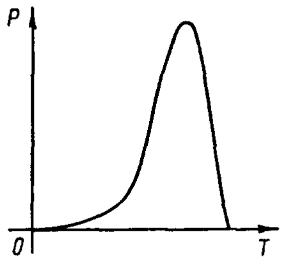

Fig. 5

Now, let the function $F(T)$ have the form shown in Fig.3 ($\tan\alpha_1 = \beta_1$, $\tan\alpha_2 = \beta_2$, $\beta_2 > \beta_1$). Then the velocity of advancement of the constant temperature $T < T_1$ should be calculated according to $\omega_1 = 2a\sqrt{\beta_1}$, and the velocity of the advancement of the constant temperature $T > T_1$ will be equal to $\omega_2 = 2a\sqrt{\beta_2}$. Since the temperature at each point rises as t increases and the higher temperatures progress more rapidly than the low ones, the higher temperatures will overtake the low. We have a situation analogous to the situation of the formation of a shock with a quite definite front. Hence, it should be considered that if the function $F(T)$ grows slowly, the flame front will be greatly extended and when $F(T)$ increases slowly for small T and rapidly for large T, the flame is characterized by a quite definite front. Furthermore, if the break point on the curve of Fig.3 is located far to the right and T_0 is significantly less than T_1, then the propagation velocity in short pipes does not succeed in attaining the value ω_2. The period of achieving the temperature T_1 in the flame may be called the period of induction. If T_1 is small or T_0 is close to T_1, the period of induction is slight. Evidently these considerations may be extended to the case of a function $F(T)$ having more than one break point.

Now, if $F(T)$ is a smooth curve such as is shown in Fig.4, then by using a piecewise linear approximation the preceding deductions may be extended to this case also and it may be considered that the propagation velocity may be calculated from Formula

$$\omega = 2a\sqrt{\beta}, \qquad \beta = \max F'(T) \tag{1.4}$$

If $F'(T)$ increases without limit, taking account of combustion then becomes essential. But the portion of the curve corresponding to values of T for which combustion is essential, may be replaced by a tangent. Combining all the above, the following conclusion may be made: if $F(T)$ has the form shown in Fig.5, the flame propagation velocity may be calculated by using (1.4).

For strongly-explosive materials the value of $\max F'(T)$ is large, and consequently, the final propagation velocity of the explosion process is large. The velocity may remain small during the period of induction.

2. The expounded one-dimensional theory does not clarify the essential effect of the magnitude of the vessel diameter on the flame propagation velocity ([5] and other papers) which is known from experiment. In order to elucidate this effect, let us consider the linearized theory of flame propagation in a semi-bounded cylinder taking into account the radial temperature distribution. The importance of taking account of radial heat propagation in the study of flame propagation has been noted in the book [6] (p.554).

We have the problem

$$\frac{\partial T}{\partial t} = a^2\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) + \beta T$$

$$T\,|_{t=0} = 0, \qquad T\,|_{r=R} = 0, \; T\,|_{x=0} = T_0 \tag{2.1}$$

where R is the pipe radius.

We may also consider a boundary condition of the form $(T_r' + \alpha T)_R = 0$.

Again setting $T = ue^{\beta t}$, we obtain

$$\frac{\partial u}{\partial t} = a^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r}\right)$$

$$u\,|_{t=0} = 0, \qquad u\,|_{r=R} = 0, \qquad u\,|_{x=0} = T_0 e^{-\beta t}$$

Let $u = X(x, t)\,\rho(r)$, then separating variables we obtain

$$\frac{d^2\rho}{dx^2} + \frac{1}{r}\frac{d\rho}{dr} + \lambda^2\rho = 0, \quad \rho\,|_{r=R} = 0 \tag{2.2}$$

$$\frac{\partial X}{\partial t} = a^2\frac{\partial^2 X}{\partial x^2} - a^2\lambda^2 X, \qquad X\,|_{t=0} = 0, \qquad X\,|_{x=0} = T_0 e^{-\beta t} \tag{2.3}$$

The functions $I_0(\lambda_n r)$, where $I_0(x)$ is the zero order Bessel function of the first kind and λ_n the roots of Equation $I_0(\lambda R) = 0$, are solutions of (2.2). Solutions of (2.3) are

$$X_n(x, t) = \frac{xT_0}{2a\sqrt{\pi}}\int_0^t \frac{\exp\left[-a^2\lambda_n^2(t-\tau)\right]}{\sqrt{(t-\tau)^3}} \exp\frac{-x^2}{4a^2(t-\tau)}\,d\tau$$

Then

$$T(x, r, t) = e^{\beta t}u(x, r, t) =$$

$$= \sum_n A_n I_0(\lambda_n r)\,\frac{xT_0}{2a\sqrt{\pi}}\int_0^t \frac{\exp\left[(\beta - a^2\lambda_n^2)(t-\tau)\right]}{\sqrt{(t-\tau)^3}} \exp\frac{-x^2}{4a^2(t-\tau)}\,d\tau$$

where the A_n are calculated from the relationship

$$\sum_n A_n I_0(\lambda_n r) = 1$$

Evidently the term corresponding to $n = 1$ is of fundamental value for large r . Hence

$$T(x, r, t) \approx A_1 I_0(\lambda_1 r) \frac{xT_0}{2a\sqrt{\pi}} \int_0^t \frac{\exp[(\beta - a^2\lambda_1^2)(t-\tau)]}{\sqrt{(t-\tau)^3}} \exp \frac{-x^2}{4a^2(t-\tau)} d\tau$$

$$(\lambda_1 = b/R)$$

Here b is the first root of Equation $I_0(x) = 0$. As in Section 1, let us consider that

$$T|_{x=0} = T_0 \quad (0 < t \leqslant t_0), \qquad T|_{x=0} = 0 \quad (t > t_0)$$

Then

$$T(x, r, t) \approx A_1 I_0(\lambda_1 r) \frac{xt_0T_0}{2a\sqrt{\pi}} \frac{\exp[(\beta - a^2\lambda_1)t]}{t^{3/2}} \exp \frac{-x^2}{4a^2t} \qquad (2.4)$$

It hence follows that if $\beta - a^2\lambda_1^2 \leqslant 0$, then $T \to 0$ as t increases, i.e. in this case the process will not be propagated. If $\beta - a^2\lambda_1^2 > 0$, then as follows from Section 1, the combustion process will be propagated with the velocity

$$\omega = 2a\sqrt{\beta - a^2\lambda_1^2} \qquad (2.5)$$

Since $\lambda_1 = b/R$ this means that the process will be damped for $R \leqslant ab/\sqrt{\beta}$ and the combustion process being propagated at a velocity $\omega > 0$ will be initiated for $R > ab/\sqrt{\beta}$

The maximum value of ω as R increases equals $2a\sqrt{\beta}$.

Let $F(T)$ have the form shown in Fig.3; then if $T_0 < T_1, R < ab/\sqrt{\beta_1}$, the flame will not be propagated in the pipe. If $T_0 < T_1$, $R_1 > ab/\sqrt{\beta_1}$, the flame first starts to be propagated at the low velocity

$$\omega_1 = 2a\sqrt{\beta_1 - a^2\lambda_1^2}$$

then, when the temperature reaches the value T_1 , a sharp increase in the flame velocity to the value

$$\omega_2 = 2a\sqrt{\beta_2 - a^2\lambda_1^2}$$

occurs.

Hence, the value $R_* = ab/\sqrt{\beta_1}$ becomes critical: for $R \leqslant R_*$ the flame is not propagated; for $R > R_*$ the flame is propagated at high velocity. As has been remarked, if the period of induction is large, the flame velocity in short pipes will be low. If $T_0 > T_1$, then a regime of propagation corresponding to the slope β_2 at once occurs. Hence, it can happen that if the diameter is less than the critical (for a value β_1), i.e. $R < ab/\sqrt{\beta_1}$, but $R > ab/\sqrt{\beta_2}$, then the combustion process does not occur for $T_0 < T_1$ but starts to be propagated at high velocity for $T_0 > T_1$.

Using reasoning analogous to that in Section 1, the case of a continuous change in the slope of the tangent and taking account of combustion may be considered. The considerations expounded above may be used to elucidate the phenomenon of the transition of combustion into detonation.

Furthermore, if $R > R_* = ab / \sqrt{\beta_1}$, then as has been remarked above, after a sufficient temperature has been achieved the flame starts to be propagated at a velocity corresponding to the slope β_2. As follows from (2.5), the flame velocity tends to the quantity $2a\sqrt{\beta_2 - \beta_1}$. as $R \to R_*$ The maximum flame propagation velocity $\omega_{max} = 2a\sqrt{\beta_2}$, and for $R \to R_*$, it becomes

$$\omega_* = 2a\sqrt{\beta_2 - \beta_1} = 2a\sqrt{\beta_2}\sqrt{1 - \beta_1/\beta_2}$$

Hence

$$\omega_* / \omega_{max} = \sqrt{1 - \beta_1/\beta_2} \qquad (2.6)$$

The dependence of the velocity ω on the coefficient of thermal diffusivity, constructed according to (2.5), is presented in Fig.6.

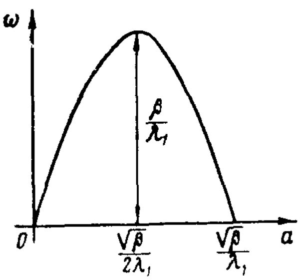

Fig. 6

At the beginning, as a increases, the velocity ω also increases to the maximum value β/λ_1, then decreases to zero. This fact is completely explainable physically since as a increases the quantity of heat being delivered through the pipe walls increases. The double role of the heat conductivity has been noted in [7] (p. 288). It can turn out that taking account of the dependence of the flame propagation velocity on the coefficient of thermal diffusivity will permit the elucidation of some peculiarities in flame propagation.

The coefficient of thermal diffusivity depends on the temperature, but also changed during the reaction in connection with the change in the concentration of the reacting materials.

Let us assume that the coefficient of thermal diffusivity depends on the temperature by increasing as the latter does. Then rapid cooling through the wall occurs on the portion where the temperature is high, the flame is quenched on this portion. The layer lying in the forefront warms up slightly during this time and starts to burn only after a certain time (the period of induction) has elapsed, etc. and pulsating combustion [5 and 7] occurs.

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