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Abstract**Full Text***Physical Chemistry*

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ON THE LIMITS OF STABLE FLAME PROPAGATION IN GASES UNDER CHANGING PRESSURE*(Presented by Academician N. N. Semenov on 9 VII 1956)*

1. In studying the mechanism of combustion by the methods of thermal theory, essential importance is attached to the role of heat transfer in the course of exothermic reactions (¹⁻³). But when the state of a gas changes at high velocities and with a large specific work, the thermal interaction (heat transfer) of the thermodynamic system with the surrounding medium is of secondary importance in comparison with the mechanical interaction (exchange of mechanical work). This is the case in combustion in pulsating-type engines, including piston engines, and in general in combustion under conditions of variable pressure and volume.

The mechanism by which flame propagation ceases (flame blowoff) is similar to the ignition mechanism: in both phenomena the basic significance belongs to the conditions of energy exchange of the reacting gas with the surrounding medium*, which determine the transition from a stationary course of reaction to a substantially nonstationary one (in ignition—from a stationary reaction accompanied by slight heating to a progressively accelerating reaction; in flame blowoff—from a stationary rapid reaction to a progressively decelerating reaction).

Questions of ignition under various forms of energy exchange with the surrounding medium were considered earlier (⁴).

2. Let us set up the energy equation for an element of the flame zone in which the reacting gases and the reaction products are located, adopting the following simplifications: a) the pressure p is the same throughout the entire volume of the chamber; b) the kinetic energy of the gases is small in comparison with their enthalpy, and therefore the change in kinetic energy is not taken into account; c) an ideal gas is considered, whose physical parameters (heat capacity, coefficient of thermal conductivity, etc.) have constant values (mean values over the interval under consideration); d) combustion (the chemical reaction) is considered as an external source of heat; e) the change in the number of moles during chemical transformations and thermal dissociation at high temperatures are not taken into account; f) a one-dimensional problem is considered, i.e., it is assumed

that the state of the gas (temperature T , density ρ , velocity u) depends on the coordinate x , whose direction coincides with the direction of flame propagation, and on the time τ .

We shall write the differential equation expressing the law of conservation of energy (the first law of thermodynamics) in the form (per unit volume per unit time):

$$c_p \rho \frac{dT}{d\tau} = \rho \frac{dQ}{d\tau} + \frac{dp}{d\tau}. \quad (1)$$

* In an analogous manner one may also treat the conditions of detonation blowoff, i.e., the transition of slow flame propagation to detonation.

Let us adopt a coordinate system fixed to the flame zone; in this coordinate system the flame zone is stationary, while the initial gas moves in the direction of the coordinate x with velocity u_{fl} . According to the condition of the problem $T = f(\tau, x)$, therefore

$$\frac{dT}{d\tau} = \frac{\partial T}{\partial \tau} + u_{fl} \frac{\partial T}{\partial x}.$$

The expression for the amount of heat supplied to a unit volume per unit time, taking into account the release of heat by the chemical reaction, heat transfer by thermal conductivity (in the direction of flame propagation), and heat transfer from the gas to the walls, may be written in the form

$$\rho \frac{dQ}{d\tau} = H_{cm} w + \lambda \frac{\partial^2 T}{\partial x^2} - \Phi_{st}.$$

Here w is the rate of the chemical reaction; H_{cm} is the thermal effect of the reaction; $\Phi_{st} = \frac{\Pi}{F} \alpha (T - T_{st})$ is the heat transfer to the walls, where α is the coefficient of heat transfer from the gas to the walls, Π is the perimeter of the flame zone, and F is its cross section.

Substituting the corresponding expressions into equation (1), dividing by $c_p \rho$, and carrying out some transformations, we obtain:

$$\frac{\partial T}{\partial \tau} + u_{fl} \frac{\partial T}{\partial x} - a \frac{\partial^2 T}{\partial x^2} = \frac{H_{cm}}{c_p} \frac{w}{\rho} + A, \quad (2)$$

where

$$A = \frac{k-1}{k} \frac{T}{p} \left[-\alpha \frac{\Pi}{F} (T - T_{st}) + \frac{dp}{d\tau} \right]$$

is a term accounting for the energy interaction of the reacting gas with the surrounding medium; $a = \lambda/c_p\rho$ is the coefficient of thermal diffusivity.

3. In application to engines, the propagation of flame in a turbulent gas mixture is of interest. Let us make certain assumptions concerning the structure of the flame zone during its propagation through a turbulent mixture.

According to modern views ⁽⁵⁾, in the case of small-scale turbulence the effect of the latter on flame propagation is associated with an intensification of the processes of heat (and mass) transfer in the flame zone, which leads to an increase in the flame propagation velocity and to a corresponding growth of the width of the flame zone ($\delta \sim u_{fl}$). Therefore, in the case of small-scale turbulence, equation (2) may with full justification be applied to a turbulent combustion zone.

To establish the conditions for cessation of flame propagation, we shall use approximate methods of solution. We shall consider the limiting case in which the rate of the chemical reaction changes very sharply with temperature (i.e. $E/RT \gg 1$) and it may be assumed ⁽²⁾ that the reaction proceeds mainly at a temperature close to the maximum combustion temperature.

Let us denote the left-hand side of equation (2) by $D(T, x)$. For $A = 0$ (i.e., for $p = \text{const}$ and $\Phi_{st} = 0$) we have from equation (2)

$$D_0 = \frac{H_{cm}}{c_p} \frac{w}{\rho}.$$

Let us denote the maximum flame temperature in the case $A = 0$ by $T_{fl.theor}$, with

$$\frac{H_{cm}}{c_p} = T_{fl.theor} - T_0.$$

Introduce the characteristic reaction time

$$\tau_r = \rho/w$$

(the time during which, at a constant reaction rate, the entire available amount of reacting substance burns out). In the case $A = 0$ we shall have $\tau_r = \tau_{r.theor}$, where

$$\tau_{r.theor} \sim e^{E/RT_{theor}}.$$

Now the preceding equation may be written in the form

$$D_0 = \frac{T_{\text{fl.theor}} - T_0}{\tau_{\text{r.theor}}},$$

where D_0 is the average rate of temperature rise in the flame zone that would result if the reaction proceeded at an unchanged rate and in the absence of heat and mass transfer, in the case $A = 0$.

Under the conditions of flame propagation at variable pressure and in the presence of heat losses to the walls, $A \neq 0$; depending on the specific

conditions it is possible that $A < 0$ and, at the same time, $D < D_0$, or $A > 0$ and $D > D_0$. Here

$$D = \frac{T_{\text{pl}} - T_0}{\tau_{\text{p}}};$$

T_{pl} is the maximum flame temperature in the case $A \neq 0$; τ_{p} is the characteristic reaction time corresponding to T_{pl} (with $\tau_{\text{p}} \sim e^{E/RT_{\text{pl}}}$).

Equation (2), in the case $A \neq 0$, may be written in the form

$$\frac{T_{\text{pl}} - T_0}{\tau_{\text{p}}} = \frac{T_{\text{pl.theor}} - T_0}{\tau_{\text{p}}} + A,$$

whence we have

$$\Delta T_{\text{pl}} = A\tau_{\text{p}}, \quad (3)$$

where $\Delta T_{\text{pl}} = T_{\text{pl}} - T_{\text{pl.theor}}$. Applying the expansion of the exponent in (3), we approximately find

$$\tau_{\text{p}} = \tau_{\text{p.theor}} e^{-\Delta T_{\text{pl}} E / RT_{\text{pl.theor}}^2}.$$

Using this expression and dividing both sides of equation (3) by $RT_{\text{pl.theor}}^2/E$, we obtain

$$\theta = \psi e^{-\theta}, \quad (4)$$

where

$$\theta = \frac{\Delta T_{\text{pl}} E}{RT_{\text{pl.theor}}^2}, \quad \psi = \frac{AE}{RT_{\text{pl.theor}}^2} \tau_{\text{p.theor}}.$$

From equation (4) we find (in studying equation (4) one may neglect the weak dependence of ψ on temperature in comparison with the exponential factor): for $A = 0$, $\theta = 0$, i.e. $\Delta T_{\text{pl}} = 0$ or $T_{\text{pl}} = T_{\text{pl.theor}}$; for $A > 0$, $\theta > 0$, i.e. $T_{\text{pl}} > T_{\text{pl.theor}}$.

In this case conditions may be created for detonation blow-off of two kinds: 1) as a consequence of ignition of the mixture* by compression (ahead of the flame front), causing the formation of shock waves; 2) as a result of the formation of shock waves associated with combustion processes in the propagating flame front.

For $A < 0$ we have $\theta < 0$, i.e. $T_{\text{pl}} < T_{\text{pl.theor}}$. Solving equation (4), one can establish that the extremal value of ψ corresponds to $\theta = -1$, i.e. the flame

temperature can decrease as a result of energy exchange by no more than the amount $RT_{\text{pl.theor}}^2/E$. We note that the same temperature drop at the limit is obtained in the case of laminar combustion at constant pressure in the presence of heat losses (2).

For $\theta \rightarrow -1$, $\partial\theta/\partial\psi \rightarrow \infty$ —a nonstationary regime occurs, accompanied by a drop in temperature and a decrease in the reaction rate, i.e. the limit of flame propagation is reached and combustion blow-off occurs.

From equation (4), after transforming it somewhat, we obtain at the blow-off boundary the approximate relation

$$\frac{[A]}{D_0} = \frac{1}{e} \frac{RT_{\text{pl.theor}}}{E},$$

i.e. the ratio $[A]$ —the magnitude of the rate of temperature decrease due to the pressure drop and heat transfer to the walls—to D_0 —the mean rate of temperature increase in the flame zone for $A = 0$ —has, at the propagation limit, a definite critical value. The presence of the factor $RT_{\text{pl.theor}}/E$ in the last expression is connected with the fact that the width of the flame zone (in which losses occur) exceeds the width of the chemical-reaction zone approximately by a factor $E/RT_{\text{pl.theor}}$.

If one introduces the characteristic time of losses

$$\tau_{\text{loss}} = \frac{RT_{\text{pl.theor}}^2}{E[A]}$$

(the time during which the gas temperature decreases by one characteristic interval owing to the change in pressure and heat transfer to the walls), then at the limit of flame propagation from equation (4) we obtain—

* Ignitions of a local character, taking into account the temperature nonuniformity of the mixture under real conditions.

we obtain $\frac{\tau_{\text{r.theor}}}{\tau_{\text{loss}}} = \frac{1}{e}$ —the ratio of the characteristic reaction time to the characteristic time of losses is constant.

4. In the case of large-scale turbulence, the combustion surface increases as a result of its deformation by turbulent pulsations; when the flame propagates, a comparatively broad combustion zone arises, having no homogeneous structure and representing, as it were, a thin flame front folded like an accordion (the layer of burning gas is divided by layers of the initial gas).

But turbulence by itself does not change the course of the chemical reaction; in the case of large-scale turbulence the reaction likewise proceeds at temperatures close to the maximum flame temperature. Therefore the constant ratio of the time of temperature decrease due to energy exchange and the time of temperature increase due to the chemical reaction ($\tau_{\text{r.theor}}/\tau_{\text{loss}} = \text{const}$), obtained as

the critical condition for blow-off of combustion in small-scale turbulence, must remain valid also for large-scale turbulence.

5. The limits of stable flame propagation depend strongly on the value of $dp/d\tau$. In the case of intermittent-combustion engines having a chamber open at one end (gas-turbine, jet engines), in determining the value $dp/d\tau$, in addition to the law of heat release, the conditions of gas flow play an important role ⁽⁶⁻⁸⁾.

In the case of piston engines $p = f(V, z)$, where $V(\tau)$ is the chamber volume, $z(\tau)$ is the fraction of the substance burned. Therefore

$$\frac{dp}{d\tau} = \left(\frac{\partial p}{\partial V} \right)_z \frac{dV}{d\tau} + \left(\frac{\partial p}{\partial z} \right)_V \frac{dz}{d\tau},$$

or, since $\left(\frac{\partial p}{\partial V} \right)_z = -k \frac{p}{V}$,

$$\frac{1}{p} \frac{dp}{d\tau} = -k \frac{d \ln V}{d\tau} + \frac{1}{p} \left(\frac{\partial p}{\partial z} \right)_V \frac{dz}{d\tau}.$$

In this equation the first term, which takes into account the change in chamber volume (motion of the piston), depends strongly on the position of the piston relative to top dead center; the second term, which takes into account burnout, depends on the thermal properties of the mixture ($H_{\text{cm}}/c_V T_0$) and on the rate of flame propagation.

Many experimental facts from the field of combustion in engines, in particular questions connected with the limits of stable operation of a piston engine with spark ignition on lean mixtures, receive a physical explanation on the basis of the considerations set forth.

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