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TRANSLATION

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Rate of Chemical Reacton and Its Effect on the Process of Droplet Combustion

by

V. R. Kuznetsov

The theory of combustion of a fuel droplet in an oxidizer stream for a purely diffusion case has been developed a long time ago [1,2]. For the general case is known only a series of qualitative results. For example, it was established that part of the fuel evaporizing in the droplet does not combust and that at certain conditions the droplet itself cannot burn [3-5].

Spaulding made an effort to explain, what these conditions are, but the baseless disregard of convective members in the heat conductivity equation led to the point, that the value V/R_0 (ratio of rate of flow coming against the droplet to its radius) during flame separation (it shows, that V/R_0-function only of the temperature of the oncoming flow) is almost a 100 times lower than the experimentally measured by Agafonova [4] and Fedoseyev [6].

In experiments [3.4] were investigated only several partial instances, by which it is impossible to make a complete picture.

The purpose of this investigation is to find a simple method, with the aid of which it would be possible to evaluate the amount of uncombusted fuel and to explain the conditions, at which the droplet cannot burn.

Agafonova [4] derived an equation, describing the process of combustion of a fuel droplet in an oxidizer stream, and formulated boundary conditions. To obtain this equation, it is necessary to assume that:

a) the boundary layer on the droplet is equivalent to a certain given film, with identical thickness everywhere,

b) the process is stationary, c) reaction is bymolecular and its rate is described by the Arrhenius equation, d) thermodiffusion and diffusional heat conductivity n be disregarded. e) $\lambda = \text{const}$, $D\rho = \text{const}$, f) $\lambda = D\rho\, c_p$.

This equation has the form of

$$\frac{d^2\theta}{d\psi^2} = K(\theta + a_1\psi + b_1)(\theta + a_2\psi + b_2)\exp\left(\frac{b}{\theta}\right) = \tilde{g}, \tag{1}$$

where

$$\theta = -\frac{c_pT}{qn_{a_1}},\quad u = \frac{v(R_0+\delta)}{D}, \tag{2}$$

$$\psi = \exp\left[-\frac{R_0^2}{(R_0+\delta)^2}\left(\frac{R_0+\delta}{R} - 1\right)\right],$$

$$b = -\frac{c_pE}{Rqn_{a_1}},$$

$$K = \frac{K_0R_0^2\left(1+\frac{2}{Nu-2}\right)^2 n_{a_1}(au_0^2)^2}{D\rho L\left(\frac{qn_{a_1}}{c_p}\right)^{1/2}(-\theta)^{3/2}\psi^2(au_0^2 - \ln\psi)^4},$$

$$a_1 = 1 - \theta_1 + \frac{l}{qn_{a_1}} + \theta_0,$$

$$a_2 = -\frac{L}{n_{a_1}} - \theta_1 + \frac{l}{qn_{a_1}} + \theta_0,$$

$$b_1 = -\frac{l}{qn_{a_1}} - \theta_0,$$

$$b_2 = \frac{L}{n_{a_1}} - \frac{l}{qn_{a_1}} - \theta_0,$$

Here T - temperature, c_p - specific heat at constant pressure, n_{a1}-concentration of oxidizer in oncoming flow, v-mass rate of substance within the film; R-current radius (read from the center of the droplet), δ - thickness of given film; D-diffusion coefficient; E-activation energy; K_0- pre-exponent, q-thermal effect of reaction by oxidizer; L - amount of oxidizer in g, necessary for the combustion of 1 g of fuel; l- specific heat of evaporation; ρ- density. The index 0 pertains to the surface of the droplet, 1- to oncoming flow.

It is assumed, that T_0- boiling point.

Boundary conditions have the form of

$$\theta|_{\psi=1} = \theta_1, \tag{3}$$

$$\theta|_{\psi=\psi_0} = \theta_0,$$

$$-\psi_0\frac{d\theta}{d\psi}\Big|_{\psi=\psi_0} = \frac{l}{qn_{a_1}}.$$

The magnitude K in the interval $[\psi_0, 1]$ varies slightly in comparison with the product of three remaining co-factors, standing in the right part of equation (1), and we will therefore consider that K = const *.

In equation (1) and in boundary conditions (3) is included an unknown parameter $u_0 r_0^2$, which cannot be determined if (1) is not first integrated. In reports [4,5] is shown, that the magnitude $u_0 r_0^2$ is proportional to the rate of evaporation, practically not differing from $(u_0 r_0^2)d$. (The index d pertains to a purely diffusional case) In conformity with this we will assume, that $u_0 r_0^2 = (u_0 r_0^2)d$. It gives

$$u_0 r_0^2 = -\frac{r_0}{1-r_0}\ln\frac{L}{\varphi n_{a_1} a_1}. \qquad (4)$$

From (3) and (4) we will obtain

$$\left.\frac{d\theta}{d\psi}\right|_{\psi=\psi_0} = -a_1. \qquad (5)$$

We will introduce a value $\eta = \dfrac{-\left.\dfrac{d\theta}{d\psi}\right|_{\psi=1}}{L/n a_1}$ equalling to the ratio of uncombusted fuel flow to the flow of evaporized fuel.

To evaluate same, we made a series of simplifications. Their validity is discussed below.

From (1) and (5) we have

$$\left.\frac{d\theta}{d\psi}\right|_{\psi=1} = -a_1 + \int_{\psi_0}^{1} \tilde{g}\,d\psi. \qquad (6)$$

We shall try finding the value of the integral in formula (6).

Since in the reaction zone the concentration of combustible components changes very sharply, and the temperature to a lesser extent, then the maximum of reproducing the concentration and maximum rate of reaction are close to each other. We will assume that they do coincide. It gives

$$\frac{d\tilde{g}}{d\psi} = 0, \quad \frac{d}{d\psi}[(\theta + a_1\psi + b_1)(\theta + a_2\psi + b_2)] = 0. \qquad (7)$$

---

* At numerical calculations values K were taken in point (θ_m, ψ_m). The index m pertains to maximum rate of chemical reaction.

$\theta + a_1\psi + b_1$ and $\theta + a_2\psi + b_2$ with an accuracy to constant multiples are equal to oxidizer and fuel concentrations respectively.

From (7) we have

$$\theta_m = c\psi_m + d, \tag{8}$$

where

$$c = -\frac{2a_1a_2}{a_1+a_2}, \quad d = -\frac{a_1b_2+a_2b_1}{a_1+a_2}. \tag{9}$$

We approximate the rate of reaction (subintegral function in (6)) by a gradual curve so as it was made by Zel'dovich and Frank-Kamenetskiy when solving the problem of normal flame propagation[7]. It gives

$$\tilde{g}(\psi) = \begin{cases} 0 & \text{при } \psi_0 < \psi < \psi_1, \\ \tilde{g}(\theta_m, \psi_m) & \text{при } \psi_1 < \psi < \psi_2, \\ 0 & \text{при } \psi_2 < \psi < 1. \end{cases} \tag{9a}$$

Assuming $\tilde{\theta}(\psi)$ - temperature distribution, corresponding to the above selected dependence $\tilde{g}(\psi)$ and satisfying the boundary conditions. To determine the $\Delta\psi = \psi_2 - \psi_1$ we employ an idea, mentioned in the above given report. In this case it leads to a relationship

$$\theta(\psi_1) - \theta_m = \theta(\psi_2) - \theta_m = \frac{\tilde{\theta}_m^2}{b}. \tag{9b}$$

The function $\tilde{\theta}(\psi)$ is approximated by two straight lines, intersecting in point (θ_m, ψ_m) and satisfying the boundary conditions (one straight line has a dip $- a_1$, and the other one $\frac{\theta_1 - \theta_m}{1 - \psi_m}$).

The interval $\Delta\psi$ and derivative $\left.\frac{d\theta}{d\psi}\right|_{\psi=1}$ is easily determined by these straight lines:

$$\Delta\psi = \frac{\tilde{\theta}_m^2}{b}\left(\frac{1}{a_1} + \frac{1-\psi_m}{\theta_1 - \tilde{\theta}_m}\right). \tag{10}$$

$$\left.\frac{d\theta}{d\psi}\right|_{\psi=1} = \frac{\theta_1 - \tilde{\theta}_m}{1-\psi_m}. \tag{11}$$

Since $\int_{\psi_0}^{1} \gamma \, d\psi = \gamma_m \Delta\psi$, then using (8) and (10), we obtain an equation for the determination of

$$\frac{K(\psi_m - \psi_{md})^3 (c\psi_m + d)^2 a_2 (a_1 - a_2)^2 (1 - \psi_m) \exp\left(\frac{b}{c\psi_m + d}\right)}{b(a_1 + a_2)(c\psi_m + d - \theta_1)} = 1 \tag{12}$$

Having found ψ_m from (12), θ_m from (8) and (12), we will obtain $\frac{d\theta}{d\psi}\Big|_{\psi=1}$ from (11). Next is found η.

Such calculations were made for an alcohol droplet in an air stream (table).

In fig.1 is given the relationship $\eta(K)$ at $\theta_1 =$ const. We investigate behavior of functions ψ_m (K) near the point ψ_d. Since the values $c\psi_m+d$, ψ_m-1, $c\psi_m+d\theta_1$ do not change much, for an approximate analysis they can be considered constant. Equation (12) acquires the form of

$$\frac{K(\psi_m-\psi_{md})^2\exp\left(\frac{b}{c\psi_m+d}\right)}{b}=\text{const.} \tag{12a}$$

At $K\to\infty$ and b = const (it corresponds to a rise in rate of chemical reaction to infinity or a reduction to zero in the rate of flow, directed around the droplet, or stoichiometric coefficient) $\psi_m\to\psi_{md}$. If the heat generating ability of the fuel or concentration of oxidizer in the stream increases, K decreases, but 1/b exp (b/cψ_m +d) rises much sharper and ψ_m also tends toward ψ_{md}.

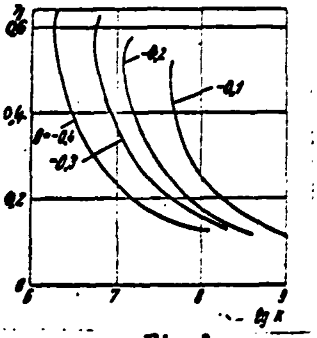

Fig.1.

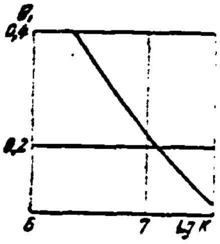

Fig.2.

Since at $\psi_m\to\psi_{md}$ from (8) $\theta_m\to\theta_{md}$ and the amount of uncombusted fuel tends to zero.

At $\psi>\psi_{md}$ $\theta+a_2\psi+b_2<0$ (negative concentration of fuel), and at $\psi<-d/c$, $\theta_m>0$, consequently $-d/c<\psi_m<\psi_{md}$.

We will now examine the conditions of flame separation. We will mention first of all that at greater values of the Nusselt criterion $K\sim R_0/V$)it is assumed, that $Nu=2+0.6\sqrt{Re}$). Consequently at unchanged temperature of oncoming flow flame separation will take place at one and the very same R_0/V values.

If we increase the rate of flow V, then the rate of evaporation will be increased. In the end there should be flame separation.

In the interval $[-d/c, \psi_{md}]$ the value

$$\frac{(1-\psi_m)(\psi_m - \psi_{md})^3 \exp\left(\frac{b}{c\psi_m + d}\right)}{c\psi_m + d - \theta_1} \qquad (12b)$$

is limited from the top, consequently at certain K values equation (12) has no solutions. The latter means that stable combustion of the droplet is impossible. The critical value K is found from formula

$$\frac{dK}{d\psi_m} = 0, \qquad (13)$$

which determines a certain curve $K(\theta_1)$, which appears to be the boundary between the zone, where stable combustion is possible, and the zone, where stable combustion is impossible. Such a curve, calculated for a drop of alcohol, burning in the flow of air, is presented in fig.2.

To check the accuracy of the approximate method of solving equation (1) was made a comparison of value $d\theta/d\psi|_{\psi=1}$ found from an accurate solution by numerical integration and found by the above explained method. Differences have not exceeded 10-15%.

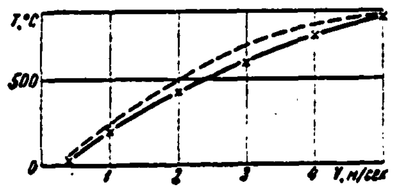

Fig.3

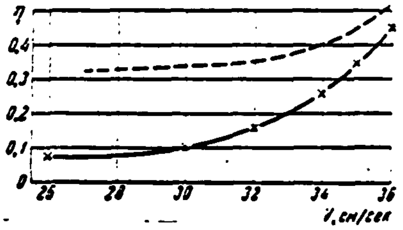

Fig.4

Calculated were also the dependences of the amount of uncombusted fuel (gasoline) upon the rate of oncoming air stream and the relationships between the temperature of the flow and its rate during flame separation.

The results of calculations are shown in fig.3 and 4 (dotted curves). For comparison on the very same figures are given experimental curves borrowed from [4].

Numerical values of magnitudes, necessary for the calculation, are given in table.

Table

Name	E.cal/mol	L	q, ккал/г	l, ккал/г	c_p, ккал/г·град	n_{O_2}	T_0,°K	K_0	$D\rho$, g.cm/sec
Ethyl alcohol	42 500	2,1	3300	220	0,33	0,23	340	$7\cdot10^{11}$	$3,2\cdot10^{-4}$
Gasoline	45 000	3,43	3000	70	0,33	0,23	365	$7\cdot10^{11}$	$1,72\cdot10^{-4}$

Greater discrepancies between values η, obtained experimentally and theoretically, are explained by failure to consider the afterburning along the path after the droplet.

The calculated dependence of the rate of the flow during flame separation upon temperature of the flow is in excellent conformity with experimental data.

Between the values V/R_0 during flame separation, obtained experimentally and theoretically, there is also satisfactory conformity (at 870° they constitute 5800 and 5600 sev^{-1}).

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