EFFECT OF THICKNESS OF FILM OF FUEL ON THE RATE OF HETEROGENEOUS (GAS—FILM) DETONATION

S. A. Lesnyak and V. G. Slutskii

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The article discusses the process of detonation in a tube filled with a gaseous oxidizer (oxygen), over whose whole perimeter there is deposited a film of fuel (a hydrocarbon with a low vapor pressure). It is assumed that the rate of heat evolution is determined by the diffusional (noninstantaneous) mixing process of the vaporizing fuel and the oxidizer. The dependence of the detonation rate on the thickness of the film of deposited fuel is obtained.

The thickness of a film of fuel, deposited on the wall of a tube filled with a gaseous oxidizer, determines the composition of a heterogeneous system. The propagation of a detonation has been observed experimentally both for very large ratios of the weights of fuel on the walls to the oxidizer in the volume, and with compositions close to stoichiometric [1, 2]. A theoretical analysis of the effect of the thickness of the film of fuel on the parameters of the detonation was made in [3, 4]. The authors assumed that the vaporized fuel entering the volume of the tube is mixed instantaneously with the oxidizer and burns. The Chapman—Jouguet plane was identified with the plane of complete vaporization of the film of fuel.

In the present article, a theoretical analysis is made of the effect of the thickness of the film of fuel on the rate of propagation of a detonation, taking account of diffusion (noninstantaneous) mixing of the vapors of the fuel and the oxidizer.

A schematic representation of the front of the detonation is shown in Fig. 1, where 0 is the shock front, x is the distance from the shock front; the arrow shows the direction of the propagation of the detonation wave. The initial thickness of the film of fuel λ_1 determines the composition of the heterogeneous system, i.e., the ratio of the weights of the fuel G_E and oxidizer G_0:

$$\varphi = \frac{1}{N}\frac{G_E}{G_0} = 4\frac{\rho_E}{\rho_0}\frac{\lambda_1}{d}\frac{1}{N},$$

where φ is the coefficient of excess fuel; N is the ratio of the weights of the fuel and the oxidizer; ρ_E/ρ_0 is the ratio of the densities of the fuel and the oxidizer; d is the diameter of the tube. Heat transfer behind the shock wave leads to vaporization of the fuel, which ends in the plane L_V. The vaporization of the fuel stops while there still remains a certain layer of fuel λ_2 on the walls of the tube. The incomplete vaporization of the film is explained by the high thermal conductivity of the metallic walls in comparison with the thermal conductivity of the gas.

In the article, the following simplifying assumptions are made: a) the density of the gas ρ, the pressure p, the temperature T, and the velocity of the flow with respect to the shock front u, are constant over the cross section of the tube and vary with increasing distance from the shock wave;

b) the ratio of the heat capacities in the flow γ is constant over the cross section of the tube, does not depend on the distance to the shock front, and is equal to the corresponding value for the detonation of a mixture of stoichiometric composition [5];

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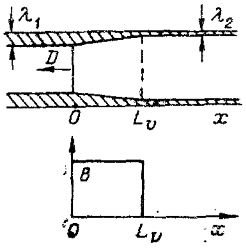

Fig. 1

c) the rate of the chemical reaction is infinitely great; the heat evolution is determined by the process of the turbulent diffusion of the fuel vaporizing behind the front of the shock wave; the concentration of fuel is variable over the cross section of the tube;

d) the value of the heat evolution per gram of reacted oxidizer H_0 does not depend on the composition of the products and is equal to the corresponding value for the homogeneous detonation of a mixture of stoichiometric composition [6]:

$$H_0 = D_H^2/2(\gamma^2 - 1)c_0', \tag{1.2}$$

where D_H and c_0' are the rate of the homogeneous detonation and the weight concentration of oxidizer in a mixture of stoichiometric composition;

e) the gas is assumed to be ideal; the parameters of state, the square of the speed of sound a^2, and the enthalpy h are connected by the relationships

$$p = \rho RT,\ a^2 = \gamma RT,\ h = a^2/(\gamma - 1),$$

where R is the specific gas constant;

f) the value of the blowing parameter $B = m/\varphi(D-u)\mathrm{St}$, where m is the rate of propagation of the shock front; St is the Stanton number, constant in the section OL_v, and equal to zero outside of it (Fig. 1). The surface of the film of fuel is assumed smooth.

In a system of coordinates connected with the shock wave, the steady-state equations of continuity, momentum, and energy, taking account of friction, heat losses, mass transfer, and heat evolution due to chemical reaction, have the form

$$\begin{gathered} S\rho u = S\rho_1 D + l\int_0^x m\,dx; \\ S(\rho u^2 + p) = S(\rho_1 D^2 + p_1) + Dl\int_0^x m\,dx + l\int_0^x \tau_w dx; \\ S\rho u(u^2/2 + h) = S\rho_1 D(D^2/2 + h_1) + (D^2/2 + h_w)\,l\int_0^x m\,dx + S\rho_1 D H_0 W + Dl\int_0^x \tau_w dx - l\int_0^x q_w dx, \end{gathered} \tag{1}$$

where S and l are the area of a tranverse cross section and the perimeter of the tube; τ_w is the tangential friction stress; q_w is the heat flux to unit surface of the film of fuel; h_w is the enthalpy of the vapors of the fuel at the surface of the film; W is the fraction of reacted oxygen; the subscript 1 relates to the starting state of the oxidizer. In (1) the quantities

$$l\int_0^x m\,dx,\quad Dl\int_0^x m\,dx,\quad (D^2/2 + h_w)\,l\int_0^x m\,dx$$

take account of the increase in the flows of mass, momentum, and energy due to the feed of the fuel; the quantities

$$l\int_0^x \tau_w dx,\quad Dl\int_0^x \tau_w dx - l\int_0^x q_w dx$$

take account of the change in the flows of momentum and energy due to friction and heat losses. With the absence of mass transfer, friction, heat losses, and chemical reaction, (1) goes over to a system of conditions at a shock wave [6].

We go over to the dimensionless coordinates and parameters:

$$\pi=p/p_1;\quad \sigma=\rho_1/\rho;\quad \mathrm{M}=u/a;\quad \mathrm{M}_1=D/a_1;$$

$$\eta_1=\int\limits_0^x \frac{lm}{S\rho_1 D}\,dx;\quad \eta_2=\int\limits_0^x \frac{l\tau_w}{S\rho_1 D^2}\,dx;\quad \eta_3=\int\limits_0^x \frac{lq_w}{S\rho_1 D^3}\,dx,$$

where π is the dimensionless pressure; σ is the dimensionless density; M is the Mach number of the flow with respect to the shock front; M_1 is the Mach number of the shock front; η_1 is the dimensionless blowing of the fuel; η_2 is the dimensionless friction; η_3 are the dimensionless heat losses. Eliminating π and σ from the equations of motion in dimensionless form, we obtain an equation of the fourth power with respect to M:

$$\gamma^2\mathrm{M}^2[\mathrm{M}^2/2+1/(\gamma-1)][\gamma\mathrm{M}^2+1]^2=(\gamma^2-Z)/2(\gamma^2-1);$$

$$Z=1-2(\gamma^2-1)\{(1+\eta_1)[(D_H/D)^2 W/2(\gamma^2-1)c_0'+(1+\eta_1)/2+(\eta_2-\eta_3][1+\eta_1+\eta_2]^{-2}-1/2\}.$$

Neglecting quantities of the order of $(\mathrm{M}_1)^{-2}$ in the expression for Z, we obtain

$$\mathrm{M}_{\pm}=\left(\frac{\gamma+1}{\gamma}\frac{1}{1\pm\sqrt{Z}}-\frac{1}{\gamma}\right)^{1/2}.$$

The plus and minus signs correspond to the two branches of the solution of Eq. (2).

An analysis of the dependence of $\mathrm{M}\pm$ makes it possible, out of all the values of the rates of propagation of the shock front, to select that value at which the process is Chapman–Jouguet detonation. To make the analysis, we need to know the dependence between η_1, η_2, η_3, W.

In the vaporization section $0L_V$, it is found possible to express the values of η_2, η_3, W in terms of the dimensionless blowing η_1 [7]:

$$\eta_1=B\frac{l}{S}\int\limits_0^x \sigma^{-1}(1-u/D)\,\mathrm{St}\,dx.$$

In actuality, assuming the validity of the Reynolds analogy

$$\mathrm{St}=c_f/2,$$

where c_f is the local friction coefficient, we obtain an expression for the dimensionless friction

$$\eta_2=\frac{l}{S}\int\limits_0^x \sigma^{-1}(1-u/D)^2\,\mathrm{St}\,dx=\langle 1-u/D\rangle\,\eta_1 B^{-1},$$

where $\langle 1-u/D\rangle$ is the mean value in the section 0x.

Assuming that, in the section $0L_V$, the whole heat flux to the surface of the fuel goes for its vaporization, we obtain

$$g_w=mr_{\mathrm{eff}},$$

where r_{eff} is the effective heat of vaporization, including the heating of the fuel up to a sufficiently high temperature and the latent heat of vaporization. In accordance with this, the expression for the dimensionless heat losses assumes the form

$$\eta_3=\eta_1 r_{\mathrm{eff}}/D^2.$$

On the basis of the experimental dependence of the distribution of the concentration of the oxidizer c_0 as a chemical element in a boundary layer with blowing and combustion above a smooth surface [8],

$$c_o/c_o^e = \left[(y/\delta)^{1/7} + (y/\delta)^{2/7} B/2\right] [1 + B/2]^{-1},$$

where c_o^e is the concentration of oxidizer at the external limit of the boundary layer; δ is the thickness of the boundary layer; y is the distance from the wall of the tube, the value of η_1 can be connected with the fraction W of reacted oxygen [7],

$$\begin{gathered}\frac{\eta_1}{1+\eta_1} = \frac{1}{S}\int\limits_{(S)} (1 - c_o)\, dS;\\ \frac{W}{(1+\eta_1)\, c_o'} = \frac{1}{S}\int\limits_{(S)} c dS;\\ c = \begin{cases} c_o/c_o', & \text{if} \quad c_o \leqslant c_o',\\ (1 - c_o)\,(1 - c_o'), & \text{if} \quad c_o \geqslant c_o'. \end{cases}\end{gathered} \tag{3}$$

These dependences, obtained for "thick" layers of fuel, hold only for the vaporization section OL_v.

In the section $L_v x$, $x > L_v$, where there is no blowing of the fuel, $\eta_1 = \eta_1^v = \text{const}$ (η_1 is the dimensionless amount of fuel vaporized in the section OL_v), it is necessary to determine the dependence between η_2, η_3, W. Since W is determined by the distribution of the concentration of oxidizer over the cross section of the tube (3), the problem reduces to seeking dependence between the change in the profile of the concentrations and the change in η_2 and η_3 with increasing distance from the plane where the vaporization of the fuel is ended.

In the section $L_v x$, the distribution of the concentration of oxygen is described by the equation

$$u\frac{\partial c_o}{\partial x} = \frac{1}{r}\frac{\partial}{\partial r}\left[r D_T \frac{\partial c_o}{\partial r}\right] \tag{4}$$

with the boundary conditions

$$\left.\frac{\partial c_o}{\partial r}\right|_{r=d/2} = 0; \quad c_o|_{x=L_v} = c_o^v, \tag{5}$$

where D_T is the coefficient of turbulent diffusion; r is the instantaneous radius of the tube; c_o^v is the distribution of oxygen in the cross section L_v. Assuming D_T constant over the cross section of the tube, from (4), (5) we obtain [9]

$$c_o = \sum_{k=1}^{\infty} A_k \exp\left[-\mu_k^2 \xi\right] J_0(\mu_k 2r/d), \tag{6}$$

where $A_k = \frac{8}{I_0^2 \mu_k d^2}\int\limits_0^{d/2} r c_o^v I_0(\mu_k 2r/d)\, dr$; μ_k are the roots of the equation $I_1(\mu_k) = 0$; I_0 and I_1 are Bessel functions of zero and first orders;

$$\xi = \int\limits_{L_v}^{x} \frac{4D_T}{ud^2}\, dx \tag{7}$$

is the dimensionless distance from the plane of the end of the mass transfer of the fuel. Thus, the change in the profile of the concentrations in the section $L_v x$ is determined by the parameter ξ. With sufficiently large values of ξ $(\xi \geqslant \mu_2^{-2})$, we limit ourselves to the two first terms of the series (6). With $\xi \leqslant \mu_2^{-2}$, we shall assume that the profile of the concentrations varies linearly with respect to ξ.

Let us determine the dependence between ξ and the change in η_2 and η_3 in the section $L_V x$. In this section, D_T is assumed constant over the cross section of the tube and equal to the coefficient of turbulent diffusion for fully developed isothermal flow in the tube [10],

$$D_T = d\sqrt{\tau_w/\rho}\,\mathrm{Sc}^{-1}/29.2 = d(D-u)\sqrt{c_f/2}\,\mathrm{Sc}^{-1}/29.2, \tag{8}$$

where Sc = 0.7 is the turbulent Schmidt number [1]]. From (7), (8) we obtain

$$\xi = \frac{1}{7.3\,\mathrm{Sc}\,d}\int_{L_v}^{x} \frac{\sigma^{-1}(1-u/D)}{1+\eta_1^v}\left(\frac{c_f}{2}\right)^{0,5} dx.$$

For the change in the value of η_2 in the section $L_V x$ we obtain

$$\eta_2 - \eta_2^v = \frac{4}{d}\int_{L_v}^{x} \sigma^{-1}(1-u/D)^2\, c_f/2\,dx = 29,2\,\mathrm{Sc}\,(1+\eta_1^v)\,\langle (1-u/D)(c_f/2)^{0,5}\rangle\,\xi.$$

Here η_2^V is the value of the dimensionless friction in the section OL_V; $\langle(1-u/D)(c_f/2)^{0.5}\rangle$ is the mean value of the quantities standing in parentheses. In the calculations made, the value of 1-u/D was assumed equal to the corresponding value in the Chapman–Jouguet plane $1-u/D \approx 1/(\gamma+1)$.

Writing the heat flux to the surface of the tube in the form [7] $q_w = \rho(D-u)\mathrm{St}H_0$ and using the Reynolds analogy St = $c_f/2$, we obtain an expression for the change in the value of η_3 in the section $L_V x$,

$$\eta_3 - \eta_3^v = \frac{4}{d}\frac{H_0}{D^2}\int_{L_v}^{x} \sigma^{-1}(1-u/D)\,\mathrm{St}\,dx = 29.2\,\mathrm{Sc}\,(1+\eta_1^v)\,\langle (c_f/2)^{0,5}\rangle\,\frac{H_0}{D^2}\,\xi,$$

where η_3^V is the value of the dimensionless heat losses in the sectio OL_V. The value of $c_f/2$ is assumed equal to the value of the local friction coefficient for flow behind a shock wave above a smooth surface $c_f/2 = \mathrm{St} = 3.7 \cdot 10^{-2}\mathrm{Re}^{-0.2}$ [12], where $\mathrm{Re} = (D-u)x/\nu$ is the Reynolds number; ν is the kinematic viscosity. Such a weak dependence of $c_f/2$ on Re determines a very weak change in the value of $(c_f/2)^{0.5}$ with increasing distance from the cross section L_V.

The dependences obtained between η_1, η_2, η_3, W make it possible to plot the dependence of $M\pm$ as a function of η_1 in the section OL_V ($\eta_1 \leqslant \eta_1^V$) and as a function ξ in the section $L_V x$. As parameters there are taken the ratio of the velocity of the shock front to the velocity of the homogeneous mixture of stoichiometric composition D/D_H, the dimensionless amount of fuel vaporized η_1^V, and the blowing parameter B.

Figure 2 shows the course of the curves for $M\pm$ for the values $\eta_1^V = 0.3$ B = 10, and different values of D/D_H. Curves 1-5 correspond to the values of D/D_H = 0.75, 0.80, 0.8166, 0.85, and 0.90. Immediately behind the shock front the flow must be subsonic and is described by the branch with the plus sign. With relatively small values of D/D_H (curve 1) the flow has a breakaway character. Physically, this means the existence of shock waves in the reaction zone, propagating toward the side of the shock front and increasing its intensity. Such a process cannot be steady-state.

With relatively large values of D/D_H (curve 5) the dependence of M_+ is continuous, but at no point does it attain a value equal to unity. The flow is found to be connected with the conditons in the initial section and can be steady-state only with a definite suppression of the combustion products.

With a single value of $D/D_H = D_j/D_H = 0.8166$ for the given values $\eta_1^V = 0.3$ and B = 10 (curve 3), the dependence of M_+ is continuous and, at the point $\xi = 0.123$, assumes a value equal to unity. The flow has a continuous character and is found to be independent of con-

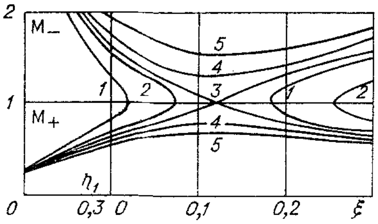

Fig. 2

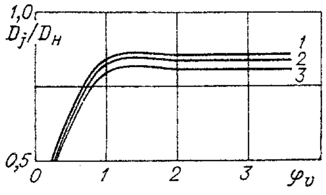

Fig. 3

ditions in the initial section of the tube: perturbations (weak rarefaction waves) from the initial section do not pass through the cross section $\xi = 0.123$, in which the Mach number of the flow with respect to the shock front is equal to zero. The propagation of the process is determined by the heat evolution, mass transfer, friction, and heat losses in the section between the shock front and the plane M = 1. Such a process will be steady-state, and the term "Chapman–Jouguet detonation" can be completely applied to it.

In an analogous manner, we can determine the value of the relative rate of heterogeneous detonation D_j/D_H and the coordinate of the Chapman–Jouguet plane (the plane M = 1) with different values of the blowing parameter B, which characterizes the vaporizability of the fuel, and the dimensionless amount of vaporized fuel, η_1^v, which characterizes the composition of the heterogeneous system.

Figure 3 shows the dependence of D_j/D_H in the form of a function of the coefficient of excess vaporized fuel

$$\varphi_v \eta_1^v/N,$$

where $\varphi_V = 1$ corresponds to a stoichiometric composition $\varphi_V < 1$ is the oxidizer contained in excess; φ_V 1 is the excess of the fuel (the overenrichments of the system). The values of the blowing parameter were B = 25, 15, and 7 (curves 1-3, respectively). Small values of B correspond to high-boiling fuels of the type of vacuum oil B ∿ 10, large values to relatively low-boiling fuels, for example, decane B ∿ 15 [7].

The results of the calculations showed that the detonation rate depends only weakly on the blowing parameters within the above limits. This permits using an approximate expression [7] for calculating B,

$$B = H_0/[c_L(T_2 - T_1) + r(T_2)]. \tag{8}$$

Here c_L, T_2, and $r(T_2)$ are the specific heat capacity, the boiling temperature, and the latent heat of vaporization of the fuel at this temperature. In (9) it is assumed that the flux to the surface of the fuel is determined by the heat evolution due to chemical reaction and goes wholly to heating the fuel up to the boiling point and to vaporization at this temperature. For "frozen" films of fuel, in the denominator of (9) account is taken of the heat of fusion and of the heating of the solid phase up to the melting point.

As follows from Fig. 3, the value of D_j/D_H does not depend on the composition of the system with $\varphi_v > \varphi_* \approx 2$. The value of φ_* corresponds to an overenriched composition in the Chapman–Jouguet plane, for detonation with rather thick layers of fuel, where vaporization also takes place beyond the Chapman–Jouguet plane. Fuel vaporization beyond the Chapman–Jouguet plane has no effect on the detonation rate.

With compositions close to stoichiometic ($1 < \varphi_v < 2$), there is only an insignificant increase in the detonation rate. Its value is approximately 20 m/sec. As is shown in [7], the defect in the rate of propagation of a detonation in the case of "thick" layers of fuel is due mainly to overenrichment of the composition in the Chapman–Jouguet plane. Therefore, an approach of the composition to stoichiometric decreases the overenrichment, thanks to which the detonation rate increases.

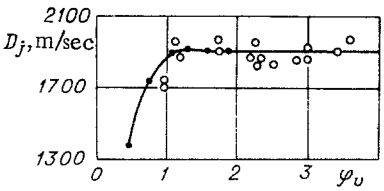

Fig. 4

Finally, with poor compositions, there is a sharp fall in the detonation rate, due to a decrease in the heat evolution.

With a comparison of experimental and calculated data, account must be taken of the fact that not all of the fuel deposited on the walls of the tube is vaporized. Part of it [a layer with the thickness λ_2 (Fig. 1)] remains on the cold metallic walls of the tube. We shall assume that vaporization of the fuel stops when the thermal boundary layer of the film of fuel reaches the walls of the tube. The thickness of the thermal boundary layer Δ is connected with the thickness of the vaporizing layer of fuel Δ_1 by the relationship [13]

$$\varkappa=\frac{\Delta}{3}\frac{d\Delta}{dt}+\frac{\Delta}{2}\frac{d\Delta_1}{dt}, \tag{10}$$

where χ is the coefficient of thermal diffusivity of the fuel; t is the time after the passage of the shock front. With application to the conditions existing with a detonation process in heterogeneous systems, from (10) it follows that the thickness of the heated layer is proportional to the thickness of the vaporized layer of fuel

$$\frac{\Delta}{\Delta_1}=k=\frac{3}{4}\left\{1-\left[1+\frac{1.8\cdot 10^4\,\varkappa\,(D_H/D)^{3.5}}{(B\Psi)^{5/4}d^{\,3/4}{p_1}^{7/4}}\right]^{0.5}\right\}. \tag{11}$$

Here $\Psi=[1+0.19(\mu_0\mu_E{}^{1/3}B]^{-1}$ is the decrease in the Stanton number due to blowing [14]; μ_E and μ_O are the molecular weights of the fuel and the oxidizer; $\varkappa$ is measured in cm^2/sec, d in cm, p_1 in atm. It can be seen from expression (11) that, with a rise in the pressure p_1 and the diameter d, the value of k tends toward zero. Since the amount of vaporized fuel is proportional to the amount of fuel deposited on the walls of the tube,

$$\varphi_v=\varphi/(1+k), \tag{12}$$

with an increase in the diameter of the tube and of the initial pressure of the oxidizer, the value of φ_V becomes close to the value of φ, characterizing the compositon of the heterogeneous system. For small-diameter tubes, with a not too great pressure of the oxidizer, the difference of k from zero must be taken into consideration.

Figure 4 gives the dependence $D_j(\varphi_V)$ for "frozen" hexadecane (B = 9.8). The value of the rate of homogeneous detonation was assumed equal to D_H = 2320 m/sec and equal to the value of the rate of the homogeneous detonation of a stoichiometic mixture of diethylcyclohexane ($C_{10}H_{20}$)—oxygen [5].

The same figure gives plots of the corresponding experimental values of the detonation rates in tubes with a diameter d = (0.475-2.22) cm with initial pressures of the oxidizer p_1 = (0.5-2) atm. The values of $D(\varphi_V)$ were calculated over from the values of $D(\varphi)$ using (12). The value of k for the above conditions was k = 0.3-1.4. There is satisfactory agreement between experimental and calculated data. Here the rate of heterogeneous detonation differs from the rate of homogeneous detonation by not less than 400 m/sec. The satisfactory agreement between the experimental and calculated data permits the conclusion that the proposed model correctly describes the effect of the thickness of the film of deposited fuel on the rate of heterogeneous detonation, if the surface of the film of fuel is smooth.

Experiments carried out with films of a liquid fuel in tubes with a diameter $d \leqslant 2.22$ cm [2] indicate a considerable difference between the experimental and calculated data. This difference can be explained by the presence of perturbations developing on the surface of a liquid fuel behind a shock wave [15], which have a considerable effect on the profiles of the concentrations and the flow parameters with such small diameters. The effect of perturbations of surface of a liqud film of combustible fuel on the detonation rate in heterogeneous systems may well be the subject of further investigations.

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