

Fig. 4

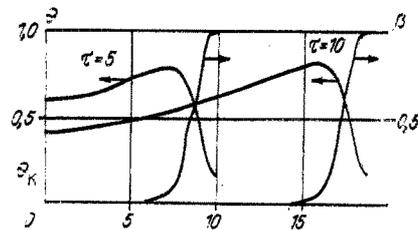


Fig. 5

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SIMPLE MODEL OF DETONATION IN A GAS-FILM SYSTEM WITH CONSIDERATION OF MECHANICAL FUEL REMOVAL

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INTRODUCTION

Many studies have been dedicated to investigations of detonation in a system consisting of a fuel film and gaseous oxidizer, for example, [1-6]. These have established the principles of detonation wave propagation in tubes of various geometry over a wide range of initial oxidizer pressures, film thicknesses, and fuel properties. For example, it was shown in [2, 3, 6] that a characteristic feature of detonation in such systems is the significant extent of the reaction zone (0.1-0.3 m) as compared to gas detonation. It has been observed experimentally [1-3] that the propagation velocity of heterogeneous detonation is much less than that of homogeneous detonation of a gas of the same composition.

Theoretical analysis of detonation structure presents significant difficulties due to the inhomogeneous flow and inhomogeneous energy liberation over the wave front. Existing models [4, 5, 7, 8] permit estimation of the wave velocity, but are not capable of predicting the length of the combustion zone and some other unique features of heterogeneous detonation. The observed reduction in heterogeneous detonation velocity as compared to gas detonation is explained by heat and momentum losses in the reaction zone. Other possible causes such as incomplete fuel mixture burnup in the reaction zone have not been considered.

Relying on the assumption of the dominant role of liquid fuel evaporation in the process of mixture formation behind the wave, [4, 5, 7] obtained a reaction zone length of ~ 1 m with stoichiometric initial composition. It was noted in [2, 9, 11] that one possible mechanism of mixture formation is destruction of the liquid film under the action of a high-velocity gas flow behind the detonation wave. Experimental studies of the behavior of liquid films behind shock waves [9-11] show that there is actually an intense process of initial fractionation of the liquid with subsequent establishment in the channel of a steady-state dispersion-ring flow with breakoff of droplets. According to the experiments of [11], the time for development of a perturbation on the surface when a shock wave passes over it ($M \sim 5$) comprises several microseconds. Viscosity of the liquid used has practically no effect on film behavior [9, 11]. The duration of heat liberation in heterogeneous detonation waves significantly exceeds such an induction period. This means that in studying processes of mixture

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formation behind detonation waves it is necessary to consider mechanical removal of liquid from the surface along with evaporation.

A shortcoming common to the existing models is their limitation to only "thin" films, i.e., films that are not disrupted by the gas flow. The approach used in [12] does not consider possible mechanisms for perturbation development on the phase boundary. Consideration of "thick" films [8] within the framework of the diffusion model which does not consider atomization of fuel would require thorough justification. In [13] a semiempirical criterion for liquid film surface stability was proposed for steady draft over the surface by a gas flow, showing that the thickness of a stable film behind a wave with Mach number 4-5 (characteristic of detonation) does not exceed several micrometers, while the surface of a film of greater thickness does not remain smooth.

Studies of the film destruction mechanism [14] show that there exists a limiting size for droplets torn from the surface (5-6 μm for water), which does not change with increase in gas velocity. Experimental observations of film destruction behind shock waves do, in fact, indicate that the droplets have a size of $\sim 10 \mu\text{m}$. Ignition of the mixture behind the wave front is apparently similar to ignition of a jet of fuel injected into a high-speed high-temperature flow of gaseous oxidizer. The droplets in such a system are so small that according to [15] they begin to evaporate before they begin burning. In the reaction zone, homogeneous combustion occurs, but because of the presence of the gas droplet layer a significant amount of fuel may not combust completely. This may cause heat liberation behind the detonation wave to be two-zone in nature, with the Chapman-Jouguet plane located in a section ahead of that in which ignition and rapid burnup of the pregenerated vapor-gas mixture occurs. Further mechanical removal of liquid from the film surface and droplet evaporation in the flow lead to slow burnup of the evaporated fuel as it mixes with the oxidizer, if the latter was not expended previously. It was shown in [4, 5] that there is a maximum in the energy liberation curve located a significant distance behind the detonation wave front. In [4, 5] the location of the Chapman-Jouguet plane was identified as the section of maximum energy liberation, without sufficient evidence.

The present study will perform an approximate calculation of steady-state detonation parameters with consideration of two mechanisms of mixture formation: mechanical removal of fuel and its evaporation.

FORMULATION OF THE PROBLEM

We will consider the motion of a steady-state detonation wave with velocity u_1 in a tube of diameter d_0 , on the wall of which there is deposited a fuel layer of thickness h_1 . The tube is filled with an oxidizer at temperature T_1 and pressure p_1 . The gas parameters ahead of the wave are denoted by the subscript 1, behind the wave, by 2, in the Chapman-Jouguet plane, by 3, on the wall surface, by w, and in the liquid, by L. The problem will be solved in a coordinate system fixed to the wave front.

Let mechanical removal of liquid from the film surface begin immediately behind the wave front, with the droplets being monodispersed with limiting size determined by the method of [14]. Since the atomized fuel consists of very fine droplets, the latter evaporate before combustion begins. In view of the low relative velocity between droplets and gas flow we will consider evaporation without convective corrections.

A study of the characteristics of fuel mixture ignition is not within the scope of the present study. No theoretical analysis of ignition of such a mixture exists in the literature, nor does systematized information on experimentally measured ignition delays over the entire range of initial system compositions. Moreover, there is a great deal of scattering between the data of various authors. For simplicity, we will assume that the fuel mixture ignites immediately after evaporation of the atomized fuel behind the wave front.

Combustion in the reaction zone is completely homogeneous. If we assume that the combustion rate is determined by the rate of supply of unreacted fuel vapor to the flame front, then analysis of energy liberation reduces to the diffusion flame model [5]. The assumptions enumerated above allow approximate description of detonation propagation in the gas-film system by the simple one-dimensional model of [5]. The model of [5] is based on modified Rankine-Hugoniot equations with losses in the reaction zone

$$\rho_1 u_1 (1 + \Phi) = \rho_3 a_3, \quad (1)$$

$$\begin{aligned}
 p_1 + \rho_1 u_1^2 (1 + \Phi) + WL &= p_3 + \rho_3 a_3^2, \\
 (i_1 + u_1^2/2) \rho_1 u_1 + \rho_1 u_1 \Phi Q + QS - QW &= \rho_3 a_3 (i_3 + a_3^2/2).
 \end{aligned}
 \tag{2}$$

Here p , ρ , T , i , u are the pressure, density, temperature, enthalpy, and velocity, respectively; Φ is the ratio of fuel mass to oxidizer mass in the tube section; WL is the momentum loss on the tube wall; QS is the work of viscous friction forces in the reaction zone; QW are thermal losses in the reaction zone; Q is the total energy of the liquid fuel which enters the reaction zone. The parameters WL , QS , and QW can be calculated with the expressions

$$\begin{aligned}
 WL &= \frac{\Pi}{A_c} \int_0^L \tau_w dx = \frac{A_s}{A_c} c_f \rho_1 u_1^2 \frac{(u_1 - u_2)^2}{2u_1 u_2}, \\
 QS &= \frac{\Pi}{A_c} \int_0^L q_s dx = \frac{A_s}{A_c} c_f \rho_1 u_1^3 \frac{(u_1 - u_2)^2}{2u_1 u_2}, \\
 QW &= \frac{\Pi}{A_c} \int_0^L q_w dx = \frac{A_s}{A_c} c_H \rho_2 (u_1 - u_2) [i_1 + (u_1 - u_2) u_1 - i_w].
 \end{aligned}$$

Here Π is the tube perimeter; A_c is the cross-sectional area; A_s is the area of the tube surface in the reaction zone; L is the length of the reaction zone; c_f and c_H are the resistance and heat liberation coefficients; τ_w , q_s , and q_w are friction, work, and thermal flux, respectively.

Equations (1) and (2) reduce to a biquadratic algebraic equation for the Mach number M_1 of the detonation wave:

$$\lambda_1 M_1^4 + 2\lambda_2 M_1^2 + \lambda_3 = 0,
 \tag{3}$$

where λ_1 , λ_2 , λ_3 are functions of the number M_1 and the parameters QS , QW , and WL . Analytical expressions for λ_1 , λ_2 , and λ_3 can be found in [5].

Equation (3) is the basis for determining the detonation propagation velocity in the gas-film system and the parameters in the Chapman-Jouguet plane by the successive approximation method. To calculate QS , QW , and WL it is necessary to define τ_w and q_w over the entire reaction zone and the reaction zone length L . Since the flow parameters behind the detonation wave change over the length of the reaction zone, simplifying assumptions are introduced. We will note only those different in form from those of [5] or added to the model.

In contrast to [5], in determining QS , QW , and WL we will commence from the condition that the liquid film surface is not smooth. The gas-liquid phase boundary is perturbed and is an irregular structure of waves and peaks with droplets breaking off. Analysis of surface wave structure using the experimental data of [10, 16, 17] shows that the ratio of wavelength to amplitude has an average value of 0.5-1.5. This fact allows consideration of the perturbed film surface as a surface with uniformly distributed dense roughness. According to [18], the thermal flux on such a surface is 1.9 times higher than on a smooth surface. Since the results of [19] indicate the approximate validity of the Reynolds analogy on the perturbed liquid surface, friction and heat exchange in the reaction zone can be defined just as in [5], but with a correction for roughness. Friction and heat exchange can be calculated on the basis of the results of [16, 17], which established a relationship between the liquid surface structure and the equivalent coefficient of a Nikuradze sand roughness.

Within the framework of a simplified analysis we will neglect jet effects, i.e., the interaction of droplets with each other. Nor will we consider the effects of droplets on processes at the wall surface. This latter assumption, necessary for calculation of the losses τ_w and q_w in the reaction zone, is applicable, since the degree of influence of droplets on processes at the film surface is determined by the size of the droplets, their number, and the duration of their stay in the boundary layer. Both the droplet size and duration of their stay in the boundary layer are small, as was noted above, and thus satisfy the assumption made.

The major difference of the model chosen for calculation of heterogeneous detonation parameters from that of [5] is the introduction of an additional mass transport mechanism in

the reaction zone: mechanical removal of liquid from the peaks of surface waves. Since the literature offers no theoretical analysis of droplet breakoff from a liquid surface with high-speed gas flows, it is desirable to use semiempirical relationships to describe the process. For example, use of the results of [19] permits writing a law of film thickness change in the form

$$\frac{dh}{dx} = - \frac{2}{\rho_L u_1} (m_v + m_E), \quad x = 0, \quad h = h_1, \quad (4)$$

where

$$m_v = [1 + 14.1(\rho_2 u_2^2)^{-0.4} (T_2/T_w)^{-0.2}] q_w/h_v, \quad (4a)$$

$$m_E = [10^{-4}(\rho_2 u_2^2)^{0.5} (T_2/T_w)^{0.25} \sigma^{-1} - 0.1] \rho_L u_w h. \quad (4b)$$

Here T_w is the film surface temperature; σ is the surface tension coefficient of the liquid fuel; u_w is the film surface velocity; h_v is the fuel's specific heat of vapor formation. In the expression for mass flow due to evaporation m_v there is a coefficient which considers intensification of turbulent heat exchange on the rough surface. In the case of a smooth surface the quantity in square brackets in Eq. (4a) is equal to unity. The expression for mass flow due to droplet breakoff m_E is derived with the assumptions of proportionality of mechanical mass removal to mass flow of the liquid in the boundary layer and linear velocity profile in the film.

Calculations of film cooling [20] indicate that mechanical liquid removal from the film surface comprises up to 80% of the total mass loss. The dependence of m_E on temperature is weak, so that for simplicity in calculations we may choose some characteristic liquid temperature for the temperature of the film surface. We will assume that the liquid has the maximum possible temperature determined by the thermal balance equation

$$q_w = m_v h_v$$

and the relation [21]

$$m_v = q_w c_w / (i_e - i_w) (1 - c_w),$$

which with use of Dalton's law gives the expression

$$\frac{h_v}{i_e - i_w} = (p_2/p_v^s - 1) M_g/M_v. \quad (5)$$

where c_w is the liquid vapor concentration on the film surface; i_e , the total gas enthalpy in the flow core; p_v^s , the saturated vapor pressure on the film surface. From Eq. (5), knowing the dependence $p_v^s(T_w)$, we can find the unknown film surface temperature.

For initial compositions $\Phi \leq \Phi^0$ we will identify the Chapman-Jouguet plane with the section in which complete evaporation of the fuel occurs (Φ^0 is the stoichiometric composition). In contrast to the model of [5], in which the Chapman-Jouguet plane is located in the section of complete evaporation of the fuel film, the approach of the present study considers not only disappearance of the film, but also complete evaporation of droplets located within the flow. Such an approach to definition of the reaction zone length only reflects the fact that the selected tube section is characteristic of the given problem. A strict approach to determination of the position of the Chapman-Jouguet plane requires consideration of the two-zone nature of energy liberation. However, due to the absence of information on ignition delays this is not possible. Within the framework of the model considered the coordinate of the Chapman-Jouguet plane gives a maximum estimate for the reaction zone length. For very thin films ($h_1 \sim 1 \mu\text{m}$) mechanical fuel removal is absent and the reaction zone length is determined by the intensity of evaporation. This means that the method of determining the Chapman-Jouguet plane coordinate proposed in [5] is a limiting case of the method proposed in the present study.

For initial compositions $\Phi > \Phi^0$ it can be proposed that the reaction zone length corresponds to the length at $\Phi = \Phi^0$. Inasmuch as we are considering a maximum estimate of

the reaction zone length here, such an assumption will imply the following. At $\Phi > \Phi^0$ within the fuel film one can always distinguish a layer the thickness of which corresponds to the "stoichiometric" thickness, i.e., the thickness at which the initial relative mixture composition $\Phi = \Phi^0$. In this case the Chapman-Jouguet plane can be identified with the section in which complete evaporation of fuel from such a layer occurs. For $\Phi \geq \Phi^0$ collision of the boundary of the moving liquid with the tube wall occurs within the reaction zone and the velocity profile in the "stoichiometric" layer is more filled than linear. Thus, Eq. (4b) gives a lowered mass removal rate, and we obtain an upper limit for the coordinate of the Chapman-Jouguet plane. For $\Phi \gg \Phi^0$ the error related to introduction of the "stoichiometric" layer with linear velocity profile is compensated by the fact that in thick films the velocity changes exponentially over thickness.

We take the fuel droplet evaporation law in the form

$$d_1^3 - d^3 = Kt,$$

where d_1 is the initial droplet diameter, d is the droplet diameter at time t ;

$$K = 8\rho_2 D_2 / \rho_L \cdot \ln(1 + B)$$

is the droplet evaporation rate coefficient [15]; D_2 is the diffusion coefficient, and B is the Spalding parameter [5].

As in [5], in determining the detonation wave parameters we will use dependences of adiabatic index γ and heat liberation per kg of mixture calculated for homogeneous detonation of a gas of the same composition.

RESULTS

The model of [5] with the above modifications was used to perform calculations by the successive approximation method for a diethylcyclohexane-oxygen mixture. The initial parameters $p_1 = (1-2) \cdot 10^5$ Pa, $T_1 = 300^\circ\text{K}$ correspond to parameters used in the detonation experiments of [2-6]. Figures 1, 3, and 4 compare the results of calculation with the model of [5], in which the only mixture formation mechanism is evaporation of liquid fuel, with the model proposed in the present study. The graphs also show experimental points obtained in [2, 3, 5, 6].

It is evident from Fig. 1 that the assumption of complete burnup in the reaction zone for $\Phi \geq \Phi^0$ is false and produces elevated steady-state detonation rates in the system. Introduction of the nonburnup coefficient k allows good description of the experimental results. Figure 2 shows the function $k(\Phi/\Phi^0)$. The fact that $k \rightarrow 0$ as $\Phi \rightarrow 0$ agrees with experimental observations. The condition $k \rightarrow 0$ corresponds to very thin films, the surface of which remains smooth upon traversal of the shock wave.

Nonburnup of the fuel mixture in the reaction zone may be a consequence of the fact that the Chapman-Jouguet plane is established at the point of completion of the ignition delay, i.e., only the energy contained in the mass of droplets accumulated up to completion of the reaction induction time is expended in maintaining the wave. In fact, if we assume that ignition delay in the system under consideration is of the same order of magnitude as the evaporation time of a droplet removed from the film surface, then calculation by Eq. (4) gives a 40-60% decrease in film thickness at a distance $l = \tau_{\text{in}} u_1$ for the condition of total mixture burnup in the reaction zone. For nonburnup $0 < k < 1$, $\tau_{\text{in}} \sim k^{-1}$, $u_1 \sim k^{1/2}$; consequently, $l \sim k^{-1/2}$. On the other hand, $m_{\text{E}}/u_1 \sim k^{1/2}$, i.e., for lower detonation rates the intensity of removal decreases in proportion to the increase in reaction zone length. Inasmuch as calculations reveal that losses in the reaction zone are insignificant, at a distance l the original film thickness decreases by a factor of approximately two due to mechanical fuel removal. This fact is in good agreement with Fig. 1, on which curve 4 best describes the experimental results of [4, 5].

Figure 3 shows curves of p_3/p_1 for various degrees of nonburnup in the reaction zone. For $\Phi \geq \Phi^0$ the model of [5] elevates the values of p_3/p_1 significantly, while for the model proposed in the present study p_3/p_1 is constant.

The model under consideration gives results for the reaction zone length qualitatively different from those of [5], which agree quite well with the corresponding experimental data, despite the approximate nature of the analysis. Measurements of the position of the Chapman-Jouguet plane by the gasdynamic criterion, employed in gas detonation for mean flow and sound

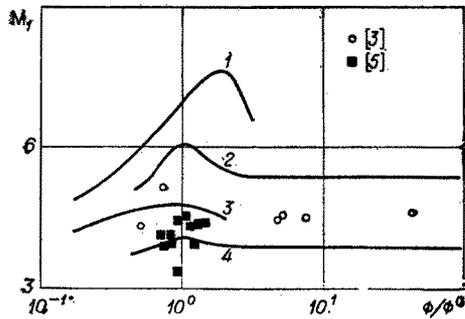


Fig. 1

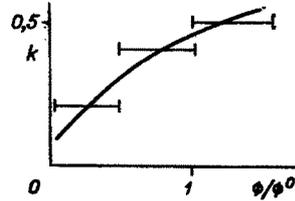


Fig. 2

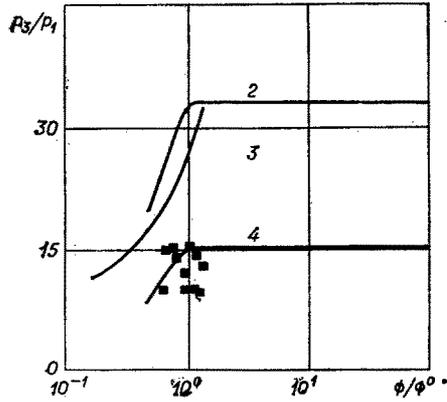


Fig. 3

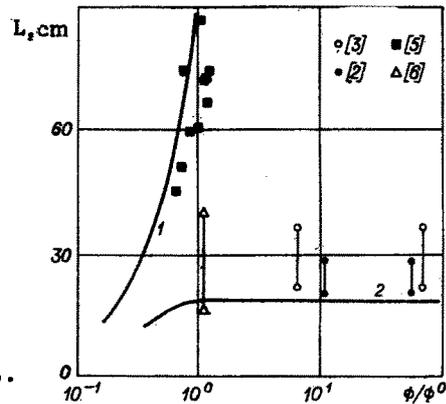


Fig. 4

Fig. 1. Detonation rate vs initial composition. 1) Homogeneous detonation; 2) complete burnup; 3) model of [5]; 4) 50% nonburnup.

Fig. 2. Nonburnup coefficient vs initial composition.

Fig. 3. Pressure in Chapman-Jouguet plane vs initial composition (notation as in Fig. 1).

Fig. 4. Reaction zone length vs initial composition. 1) Model of [5]; 2) 50% nonburnup.

velocities over tube sections, as carried out in [6], are more valid than the heat liberation profile measurements of [4, 5]. The experimental data of [4, 5] noted in Fig. 4 show that the maximum in heat liberation is located further from the wave front, the larger Φ . It is evident that this is due to the fact that at large Φ the system is more inhomogeneous and burnup of the fuel mixture occurs later. The experimental points from [2, 3] correspond to the distance at which the flame closes in upon the center of the tube, and is practically independent of Φ . The data from [6] are shown in Fig. 4 in the form of maximum and minimum estimates ($L_{\max} = 10d_0$, $L_{\min} = 4d_0$). The decrease in the reaction zone length in the present analysis can be explained as due to the introduction of an additional mixture formation mechanism — mechanical mass removal. This leads to an approximate relationship between the results for $\Phi < \Phi^0$:

$$L_{E+v}/L_v \sim (1 + m_E/m_v)^{-1},$$

where L_{E+v} is the reaction zone length in the present mode and L_v is that in the model considering only fuel evaporation. It is evident from Fig. 4 that mass removal due to droplet breakoff remains the main mixture formation mechanism over a wide range of initial system compositions.

The character of the change in $L(\Phi/\Phi^0)$ (Fig. 4, curve 2) is to some degree explainable by the absence of a rich limit for detonation propagation and is in accord with [3]. It should, however, be noted that for each tube there exist initial oxidizer pressures such that the film

is blown from the tube wall practically immediately after the wave front. Under such conditions the droplets fill the entire tube section and the system is so overrich with fuel that detonation may not set in.

The character of curve 2 in Fig. 4 is determined mainly by Eq. (4b). Obtained for film cooling calculations, it gives satisfactory results. However, for a detailed study of heterogeneous detonation in a gas-film system a systematic analysis of the development of instability and droplet breakoff under high-velocity flow conditions following shock and detonation waves will be required. The proposed model can be used as a starting point for creation of a strict quantitative model of heterogeneous detonation.

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