DETONATION REACTION ZONE IN TWO-PHASE MIXTURES

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The dynamics of compression wave propagation in two-phase gas-liquid fuel mixtures is of great interest in view of the widespread use of atomized liquid fuels in various types of combustion chambers. The most important of the questions relation to the study of compression wave propagation in such mixtures are:

a) the mechanism of amplification of the compression waves as they travel through the burning twophase system;

b) the conditions governing the transition from combustion to detonation.

The study of the detonation of two-phase mixtures is also interesting in that in such systems it is possible, in principle, to obtain detonation waves intermediate in intensity between the detonation waves in gases and condensed explosives.

Since the rate of heat release in the detonation waves of two-phase mixtures must be chiefly determined by the rate of transition from the liquid to the gas phase, which is only weakly temperature-dependent, in these systems, as distinct from a gas detonation, the temperature in the reaction zone should vary smoothly without an induction period and a subsequent sharp rise.

In this case the width of the heat release zone will depend only weakly on the thermodynamic and hydrodynamic parameters behind the wave and their fluctuations. Heterogeneous detonation waves are therefore apparently less susceptible to distortion of flow one-dimensionality due to instability of the shock wave-ignition zone complex.

In studying the process of transition from combustion to detonation and the nature of the detonation limits in two-phase mixtures it is important to determine the extent of the reaction zone, it is possible to judge between the Jouguet point and the shock front. From the extent of the reaction zone it is possible to judge the energy fraction going to sustain the wave and the heat losses to the walls of the channel, through which the detonation wave is propagated.

It follows from the above that, apart from assisting with the solution of practical problems, the investigation of two-phase detonating mixtures can supply valuable information of a theoretical nature relating to the wave structure, the detonation limit, and the nonstationary processes associated with the passage of compression and shock waves through a burning two-phase mixture.

The existence of detonation waves in mixtures consisting of liquid droplets atomized in a gaseous oxidizer was experimentally demonstrated in [1-4], where the amplification of fairly weak shock waves (Mach number $M \approx 1.1$) on passing through regions filled with burning droplets was also detected. The pos-

*By the reaction zone in a two-phase mixture we understand the zone in which the chemical reactions involving heat release take place. The width of the reaction zone (or heat release zone) and the reaction rate may be determined by the rate of any of the physical or chemical processes taking place in the gas-liquid mixture.

Moscow. Translated from Fizika Goreniya i Vzryva, Vol. 6, No. 3, pp. 374-385, July-September, 1970. Original article submitted November 26, 1968.

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sibility of detonation in two-phase sprays with a low liquid-phase volume content was analyzed theoretically by Williams [5], who concluded that in such systems detonation is possible if:

a) for heat release controlled by the rate of vaporization the droplet size does not exceed 10 μ (such small droplets have a very high rate of vaporization);

b) for larger droplets heat release is controlled by the more rapid process of gasification by breakup of the droplets in the flow behind the wave. The authors of [1-4], analyzing the experimental data obtained, concluded that breakup of the droplets has a decisive effect on the propagation of detonation in a two-phase droplet mixture. This is particularly clearly demonstrated in [4].

Qualitatively, the amplification of compression waves and detonation in burning two-phase mixtures can be represented in the following form. After passage of the compression wave through a volume element of the mixture owing to the inertia of the liquid a gasdynamic relaxation zone, in which momentum transfer between the gas and the droplets takes place, is formed. Since the droplets are exposed to a high-velocity gas flow, they become unstable, their surface is distorted, and extremely fine droplets which vaporize almost instantaneously separate from the surface [6]. The process of transition from the liquid to the gas phase (mass release) is also sharply intensified if there is a sufficient amount of the other component in the neighborhood of the disintegrating droplet; at a sufficiently high temperature there may be an increase in burning rate accompanied by a local rise in pressure behind the starting wave. Under certain conditions the new waves created by the local pressure rise may overtake and amplify the first compression wave. Since droplet breakup and hence heat release depend on the velocity of the gas behind the compression wave, wave amplification will be progressive. Thus, if the wave takes a sufficiently long time to pass through the burning mixture a detonation wave may develop. Unfortunately, we are still unable to obtain a complete and exact solution of the nonstationary problem of the propagation of an arbitrary compression wave in a burning two-phase mixture. This is associated both with the lack of experimental data on the behavior of compression waves in burning two-phase mixtures and with our ignorance of two-phase flow behavior behind a shock front in the presence of mass and heat release.

We have investigated the variation of the thermodynamic and gasdynamic parameters of a mixture in the reaction zone of the detonation wave. Our object was to estimate the width of the heat release zone behind the wave, which is a criterion of the possibility of detonation and steady-state propagation, in chambers with a specific geometry. A further object of the investigation was to obtain theoretical curves for the heat release in the reaction zone for various possible vaporization mechanisms, in order to be able to determine from a comparison with experiment which process controls the rate of heat release in actual detonation waves in two-phase mixtures.

Formulation of the Problem

We will consider a fuel mixture consisting of droplets of liquid fuel uniformly distributed in a gaseous oxidizer atmosphere. Through this mixture a one-dimensional plane detonation wave is propagated at velocity u_0 . We describe the motion of the medium in coordinates tied to the leading front of the detonation wave, whose location is characterized by the value x = 0; the x axis is directed away from the front in the direction of the combustion products. The state of the mixture ahead of the wave front is described by the following parameters: p_0 is the gas pressure; T_0 is the temperature; ρ_0 is the density of the gas phase; σ_0 is the mass liquid-fuel concentration; d is the liquid density; r_0 is the radius of the liquid droplets; u_0 is the gas velocity; and w_0 is the droplet velocity (obviously, $u_0 = w_0$). The values of these parameters in the reaction zone are detonated by the same letters but without subscripts.

The principal assumptions made in deriving and solving the equations are as follows:

1) the liquid droplets are nondeformable spheres of the same radius that do not coalesce or collide with each other;

2) the distances on which the flow parameters change significantly are large as compared with the dimensions of the droplets;

- 3) the volume occupied by the droplets is negligibly small as compared with the volume of the gas;
- 4) viscosity and thermal conductivity are important only in phase interaction processes;
- 5) the structure of the detonation wave corresponds to the ideal Zel'dovich-Neumann-Doering model,

i.e., the detonation wave is a stable stationary complex consisting of a shock wave with a subsequent deflagration zone, in which the starting components are converted to combustion products.

The first four of these assumptions are customary in connection with two-phase flow, while the last is typical of most detonation studies.

In analyzing the processes of mass and heat release we will consider two models:

1) the rate of heat release is wholly determined by the rate of the droplet evaporation process;

2) the rate of heat release is determined by the rate of droplet breakup.

In the first model the entire mass of evaporated material is instantaneously burned, i.e., it is assumed that the mixing of the components and their reaction proceed at infinitely high rates. The second model presupposes that the mass of the microdroplets separated from the main disintegrating droplet instantaneously evaporates and reacts with the oxidizer. In other words, the rate of combustion and evaporation of the mist formed as a result of droplet breakup in the high-velocity flow is much greater than the rate of conversion of the liquid from droplet to mist. In the case in question the temperature of the gas behind the shock wave is about 2000°K. At such temperatures the ignition lags of a heptane-oxygen mixture should be less than 10^{-6} sec; consequently, the assumption of an infinitely high reaction rate will be well satisfied for waves in which the heat release zone is a few millimeters or more wide. Although we lack data on the vapor-oxidizer mixing rates in the path of a droplet in a supersonic flow, it is reasonable to suppose that the width of the mixing zone does not exceed a few droplet diameters. Consequently, mixing will limit the burning rate only when the heat release zone in the wave is of the order of the droplet diameter. A detailed analysis of the conditions under which the assumptions underlying the above two models are satisfied may be found in [7,8].

The evaporation time of the microdroplets separating from the main droplet is of the order of 1μ sec. In fact, in the presence of the large dynamic heads that exist in detonation waves they do not exceed 1μ in size [9], and for the values of the flow parameters adopted below, the evaporation zone of such droplets will not extend over more than 1 mm. Consequently, the conditions of model 2 will be satisfied for detonation waves in which the heat release zone extends over a few millimeters or more.

In order to simplify the calculations we assume that the droplet temperature is constant and disregard the deformation of the droplets during breakup. In reality, the droplets are deformed in the flow, but while taking this deformation into account may slightly modify the quantitative results it does not fundamentally affect the qualitative character of the relations obtained. The assumption that the droplet temperature is constant implies that all the heat reaching the droplet is expended on evaporation. This condition does not impose any serious limitations on the applicability of the solution obtained below.

We also neglect the temperature dependence of the viscosity and surface tension of the liquid and the viscosity of the gas.

Basic Equations. In our case the equations of motion of a two-phase medium may be written as follows: continuity

$$\rho u + \sigma w = \rho_0 u_0 + \sigma_0 w_0; \tag{1}$$

conservation of momentum

$$\rho u^{2} + \sigma w^{2} + p = \rho_{0} u_{0}^{2} + \sigma_{0} w_{0}^{2} + \rho_{0}; \qquad (2)$$

conservation of energy

$$\rho \, u \left[\frac{\gamma \, \rho}{(\gamma - 1) \, \rho} + \frac{u^2}{2} \right] + \sigma \, w \left[c \, T_0 + Q + \frac{w^2}{2} \right]$$

$$= \rho_0 \, u_0 \left[\frac{\gamma_0 \, \rho_0}{(\gamma_0 - 1) \, \rho_0} + \frac{u_0^2}{2} \right] + \sigma_0 \, w_0 \left[c \, T_0 + Q + \frac{w_0^2}{2} \right]. \tag{3}$$

Here, c is the specific heat of the liquid; γ is the ratio of specific heats c_p/c_v for the gas phase; and Q is the heat of combustion of the fuel.

The mass concentration of the liquid can be represented by the following equation:

$$\mathfrak{s}=\frac{4}{3}\,\pi\,r^3\,n\,d,$$

where n is the number of droplets per unit volume. Since we have assumed that the droplets do not coalesce and that the microdroplets forming the mists burn instantaneously, the droplet flux is a constant quantity, i.e.,

$$n\omega = \text{const.}$$
 (4)

The equation of state of the gas phase is written

$$p = \frac{\rho R T}{M},\tag{5}$$

where M is the mean-molecular weight of the gas; and R is the universal gas constant. Apart from the conservation laws, in order to take into account mass, momentum, and energy transfer between the phases it is necessary to use two additional equations: the equations of motion and mass decrease of the droplets. The first of these is the aerodynamic drag-force equation

$$\sigma w \frac{d w}{d x} = \frac{C_x \rho (w - u) |w - u| \pi r^2}{2}.$$

where C_X is the drag coefficient which in accordance with [10] can be expressed as a function of the Reynolds number

$$C_{x} = \begin{cases} 27 \text{Re}^{-0.84} & \text{at} \quad \text{Re} < 80, \\ 0.27 \text{Re}^{0.21} & \text{at} \quad 80 < \text{Re} < 10^{4}, \\ 2 & \text{at} \quad \text{Re} > 10^{4}. \end{cases}$$
(7)

Here, Re = 2 $[r(w - u)/\nu_g](\nu_g)$ is the kinematic viscosity of the gas). The form of the second auxiliary equation depends on the choice of the process limiting the rate of mass transfer from the liquid to the gas phase. When the mass decrease of the droplet is determined by evaporation [11]

$$w \frac{dr}{dx} = -k' \frac{Nu}{16r}, Nu = \frac{2rh}{\lambda},$$
(8)

where k' is the evaporation coefficient; Nu is the Nusselt number; h is the heat transfer coefficient; and λ the thermal conductivity. In computing the Nusselt number it is possible to use the Ranz-Marshall equation [11]:

$$Nu = 2 + 0.53 Re^{0.5}$$
.

There are several expressions for describing the law of mass decrease of a disintegrating droplet. In what follows we employ the two which, in our opinion, most accurately describe the dependence of the liquid-gas conversion rate on the flow parameters and the properties of the liquid and the gas.

The first of these was proposed by Engel [12] and takes the form

$$w \frac{d v}{d x} = -4\pi \left(\frac{v g}{v l}\right)^{1/6} \left(\frac{\rho}{d}\right)^{1/3} v_{l}^{0.5} (w-u)^{0.5} r^{1.5}, \qquad (9)$$

where v is the volume of the droplet; and η is the kinematic viscosity of the liquid.

The second law of mass decrease was proposed by Priem [8]; in this case

$$w \frac{d m}{d x} = \frac{m_0}{\tau_{\rm b}},\tag{10}$$

where m_0 is the initial mass of the droplet; m is the variable mass; and τ_b , the disintegration time, is equal to [8]

$$\tau_{\rm b} = 6,43 \left(\frac{d}{\rho}\right)^{1/3} \left(\frac{{}^{\nu}{\rm g}}{{}^{\nu}{\rm g}}\right)^{1/3} \frac{r \cdot {\rm Re}^{0.75}}{(w-u) (2{\rm We})^{0.5}}.$$
(11)

Here, We = $[\rho(w-u)^2 2r/\Psi]$ is the Weber number; and Ψ is the surface tension of the liquid.

Denoting all the variables immediately behind the shock front by the subscript 1, we introduce these dimensionless variables:

$$\overline{w} = \frac{w}{w_0}, \quad \overline{u} = \frac{u}{u_0}, \quad \overline{\sigma} = \frac{\sigma}{\sigma_0}, \quad \overline{r} = \frac{r}{r_0}, \quad \overline{n} = \frac{n}{n_0}, \quad \overline{x} = \frac{x}{r_0},$$
$$\overline{p} = \frac{p}{p_1}, \quad \overline{T} = \frac{T}{T_1}, \quad \overline{\rho} = \rho/\rho_1.$$

Equation (1) now becomes

$$\bar{u} = \frac{\rho_0}{\rho_1} \frac{1}{\rho} \left[1 + \frac{\sigma_0}{\rho_0} \left(1 - \hat{\sigma} \, \widetilde{w} \right) \right], \tag{12}$$

and Eq. (2)

$$\boldsymbol{p}_{1}\,\boldsymbol{\tilde{p}}=1+\frac{\rho_{0}\,\boldsymbol{u}_{0}^{2}}{\rho_{0}}\left\{1+\frac{\sigma_{0}}{\rho_{0}}\left(1-\overline{\sigma}\,\overline{\boldsymbol{w}}^{2}\right)-\frac{\rho_{0}}{\rho_{1}\,\overline{\rho}}\left[1+\frac{\sigma_{0}}{\rho_{0}}\left(1-\overline{\sigma}\,\overline{\boldsymbol{w}}\right)\right]^{2}\right\}.$$
(13)

Using Eqs. (12) and (13) and the energy conservation equation, we express the dimensionless density of the of the gas phase in terms of the droplet velocity and the degree of combustion $1 - \sigma \overline{w}$.

$$\bar{\rho} = \frac{\rho_{0} \left[1 + \frac{\sigma_{0}}{\rho_{0}} \left(1 - \bar{\sigma} \, \overline{w} \right) \right] \left[\frac{\rho_{0}}{\rho_{0} u_{0}^{2}} + 1 + \frac{\sigma_{0}}{\rho_{0}} \left(1 - \bar{\sigma} \, \overline{w}^{3} \right) \right] \frac{\gamma}{\gamma - 1}}{\rho_{1} \left\{ \frac{2\gamma_{0} \rho_{0}}{(\gamma_{1} - 1) \rho_{0} u_{0}^{2}} + 1 + \frac{\sigma_{0}}{\rho_{0}} \left[\frac{2(c T + Q)}{u_{0}^{2}} \left(1 - \bar{\sigma} \, \overline{w} \right) + \left(1 - \bar{\sigma} \, \overline{w}^{3} \right) \right] \right\}}; \\ \left\{ 1 + \sqrt{1 - \left[\frac{1 + \frac{\sigma_{0}}{\rho_{0}} \left(1 - \bar{\sigma} \, \overline{w} \right) \right] \left\{ \frac{2\gamma_{0} \rho_{0}}{(\gamma_{0} - 1) \rho_{0} u_{0}^{2}} + 1 + \frac{\sqrt{\rho_{0}}}{\left[\frac{\rho_{0}}{\rho_{0} u_{0}^{2}} + \frac{1 + \bar{\sigma}_{0}}{\left[\frac{\rho_{0}}{\mu_{0} u_{0}^{2}} + \frac{1 + \bar{\sigma}_{0}}{\left[\frac{2(c T + Q)}{u_{0}^{2}} \left(1 - \bar{\sigma} \, \overline{w} \right) + 1 - \bar{\sigma} \, \overline{w}^{3}} \right]} \right\}} + \left[1 + \frac{\sigma_{0}}{\rho_{0}} \left(1 - \bar{\sigma} \, \overline{w}^{3} \right) \right] \right\}^{2} \frac{\gamma^{2}}{\gamma^{2} - 1}},$$
(14)

This expression can be simplified somewhat if we consider that in the detonation zone

$$\frac{p_0}{\rho_0 u_0^2} \ll 1$$

while in the Chapman-Jouguet plane, the radicand should vanish. As in ordinary gas detonation, we assume that the gas velocity behind the wave and the speed of sound are equal at a point where the energy has been completely released, i.e., $\sigma = 0$. The equation obtained from this condition $(1 + \sigma_0/\rho_0) \gamma_2^2/\gamma_2^2 - 1 = (2\gamma_0/(\gamma_0 - 1)) (p_0/\rho_0) + 1 + \sigma_0/\rho_0 + (\sigma_0/\rho_0)[2 (cT + Q)/u_0^2]$ can be used to eliminate Q + cT from Eq. (14). Here, γ_2 is the ratio of specific heats in the detonation products. For simplicity it has been assumed that γ varies linearly as the fuel is consumed:

$$\gamma = \gamma_1 - (1 - \overline{\sigma w}) (\gamma_1 - \gamma_2).$$

We write the remaining equations in dimensionless form:

equation of state

$$\bar{p} = \frac{\bar{p} \bar{T}}{\bar{M}}, \qquad (15)$$

where $\overline{M} = M/M_T \approx 1$;

conservation of the total number of droplets

 $\overline{n w} = 1$ (16)

at

$$\bar{\sigma} = \tilde{n} \, \bar{r}^3; \tag{17}$$

equations of motion of the droplets:

$$\overline{w} \frac{d \overline{w}}{d \overline{x}} = -A_1 \frac{(\overline{w} - \overline{u})^{2,21} \overline{\rho}}{(\overline{\sigma} \overline{w})^{0.26}} \quad (80 < \text{Re} < 10^4),$$
(18)

$$\overline{w} \frac{d \overline{w}}{d \overline{x}} = -A_2 \frac{(\overline{w} - \overline{u})^{1.16} \overline{\rho}}{(\overline{\sigma} \overline{w})^{0.61}} \quad (\text{Re} < 80);$$
(19)

mass variation of the evaporating droplet

$$\overline{w} \frac{d\left(\overline{\sigma} \ \overline{w}\right)}{d \ \overline{x}} = - \left[B_1 \left(\overline{\sigma} \ \overline{w}\right)^{0.33} + B_2 \left(\overline{w} - \overline{u}\right)^{0.5} (\overline{\sigma} \ \overline{w})^{0.5} \right]; \tag{20}$$

Engel's mass decrease equation

$$\frac{\overline{w} \ d \ (\overline{\sigma} \ \overline{w})}{d \ \overline{x}} = -C_1 \ (\overline{w} - \overline{u})^{0.5} \ \overline{\rho}^{0.33} \ (\overline{\sigma} \ \overline{w})^{0.5}$$
(21)

Priem's mass decrease equation (linear law)

$$\overline{w} \frac{d(\overline{s} \ \overline{w})}{d \ \overline{x}} = -C_2 \frac{(\overline{w} - \overline{u})^{1.25} \ p^{0.85}}{(\overline{s} \ \overline{w})^{0.41}}.$$
(22)

The constant coefficients in Eqs. (17)-(22) are expressed in the form

$$A_{1} = \frac{3}{8} \cdot 0.27 \operatorname{Re}_{0}^{0.21} \frac{\rho_{1}}{d}; \quad A_{2} = \frac{3}{8} \frac{27}{\operatorname{Re}_{0}^{0.84}} \cdot \frac{\rho_{1}}{d};$$
$$B_{1} = \frac{3}{8} \cdot \frac{k'}{u_{0} r_{0}}; \quad B_{2} = \frac{1,59}{16} \frac{k' \operatorname{Re}_{0}^{0.5}}{u_{0} r_{0}};$$
$$C_{1} = 3 \sqrt{2} \left(\frac{\rho_{1}}{d}\right)^{0.33} \operatorname{Re}_{0}^{-0.5} \left(\frac{\sqrt{l}}{\sqrt{g_{1}}}\right)^{0.33};$$
$$C_{2} = \frac{\sqrt{2} (\operatorname{We}_{0})^{0.5} \operatorname{Re}_{0}^{-0.75}}{6,43} \left(\frac{\rho_{1}}{d}\right)^{0.33} \left(\frac{\gamma_{1}}{\sqrt{g_{1}}}\right)^{0.33};$$

where

$$\operatorname{Re}_{0} = \frac{2r_{0} u_{0}}{v_{g1}}, \ \operatorname{We}_{0} = \frac{\rho_{1} u_{0}^{2} 2r_{0}}{\psi}$$

As may be seen from the equations, in order to find all the parameters of the two-phase mixture behind the wave front as functions of the x coordinate it is necessary to solve a system of two differential equations, in which the variables are σ and \overline{w} . The other parameters of the mixture are expressed algebraically in terms of σ and \overline{w} .

Principal Results of the Calculations

No pair of differential equations (17)-(22) describing the behavior of the droplets in the flow behind the wave can be solved analytically, since all the equations are nonlinear differential equations with inseparable variables. A solution was obtained numerically on a Mir computer using a finite-difference method with variable integration step. The integration step decreased automatically as $(w - u) \rightarrow 0$, so that the difference $(\overline{w} - \overline{u})$ always remained positive. The two-phase system for which the calculations were made consisted of heptane droplets and oxygen gas. For ideal conditions and a stoichiometric composition the detonation velocity in this mixture is 2400 m/sec [3]. The initial temperature of the droplets and the oxygen $T_0 =$ 300° K, and the pressure $p_0 = 1$ atm. For a stoichiometric composition the ratio $\sigma_0/\rho_0 = 0.284$. We investigated three variants of a monodisperse heptane spray in oxygen with droplet size $r_0 = 10$, 100, 1000 μ . The values of the thermophysical parameters of the liquid and the gas used in the calculations are given in Table 1.

In the course of the numerical integration the value of the Reynolds number was continuously checked to ensure that the expression for the drag coefficient in the equation of motion of the droplet corresponded to the given R_{e^*} . In calculating the breakup of the droplets we also checked the Weber number. The calculations were interrupted when $We \leq We_{cr} = 100$. The choice of the value $We_{cr} = 100$ was determined by the characteristics of the actual droplet breakup mechanism. As many droplet breakup studies have shown, at $We \geq 100$ a surface layer of liquid separates from the droplet owing instability in the high-velocity flow and, at the same time, the droplet is deformed. However, as long as the deformation does not reach the

| | Parameter | | | | | | | |
|-------------------------------|-----------|------------|-----|---------------------|-----------------------------|---|----------------------|----------|
| Substance | To | Τ ι | T2 | ψ N/m | ρkg/m ³ kg/sec.m | | m²/sec | P1/P0 |
| Oxygen · · · Heptane · · · | 1,4 | 1,3 | 1,2 | 20·10 ⁻³ | 1,3 675 | 20,7.10 ⁻⁶ 370.10 ⁻⁶ | 2,7·10 ⁻⁶ | 6,9 — |

| ΤA | В | I | \mathbf{E} | 1 |
|----|---|---|--------------|---|
| | | | | |

TABLE 2

| | Coefficient | | | | | | | | |
|-------------------------------------|---------------------|---------------------|---------------------|----------------------|----------------------|----------------------|--|--|--|
| r0, M | $A_1 \cdot 10^3$ | $A_2 \cdot 10^7$ | B1+107 | B2+104 | C1.104 | $C_2 \cdot 10^3$ | | | |
| 10^{-3} 10^{-4} 10^{-5} | 2,95 1,77 1,1 | 6,61 45,7 316 | 4,23 42,3 423 | 1,61 5,09 16,1 | 4,32 13,7 43,1 | 1,33 2,42 4,23 | | | |

critical stage in which the droplets are converted into perforated disks, the mass release from the disintegrating droplet is satisfactorily described by the equations presented above. In the general case the droplets, especially the large ones, are not able to lose all their mass during the deformation period (as which we may take, for example, the time required for the upstream and downstream surfaces of the droplet to coalesce [13]). As a result of the intense deformation the remainder of the droplet breaks down into smaller individual droplets. Unfortunately, there are no expressions for the vaporization rate in this stage of disintegration; accordingly, the computations were continued only as long as the droplet decreased in mass while always remaining a single entity. Although the condition We = 100 is not equivalent to the condition of loss of droplet integrity, as numerous calculations show, they correspond quite well.

The coefficients calculated on the basis of the above values of the parameters of the liquid and the gas and used in basic equations (17)-(22) are given in Table 2.

The principal results of the numerical calculation of the parameters of the two-phase flow behind the detonation front are presented in Figs. 1, 2, and 3.

An analysis of the three cases considered leads to the conclusion that the heterogeneous detonation reaction zone is longer than the reaction zone that the detonation wave in a mixture of the same components would have if they were both gaseous. When the burning rate is determined by the evaporation of the liquid fuel, only part of the fuel (an especially small part in the case of large droplets) is able to burn before the gas and droplet velocities are equalized. Subsequently, combustion proceeds according to the even slower law $r_0^2 - r^2 = k't$ (k' is the evaporation coefficient and t,time). An estimate of the distance on which the droplets should be completely vaporized gives a value $x \approx 6$ m. It follows from Fig. 1 that the droplet size has a strong influence on the flow parameters behind the wave front. Whereas for droplets with a radius of 10 μ at a distance x = 3 mm from the front about 45% of the initial mass has been consumed, for droplets with a radius for 1000 μ at the same distance the consumed mass fraction is scarcely 1%.

The principal parameters of the two-phase flow for the case when the burning rate is determined by the rate of droplet disintegration are presented in the form of graphs in Figs. 2 and 3, from a comparison of which it follows that the two droplet disintegration laws give similar results.

The comparison of the $\overline{\sigma w} = g(x)$ curves for the disintegration and evaporation models demonstrates clearly how the combustion process is intensified by the breakup of the fuel droplets. For the finest droplets the burnup process ends before the gas and droplet velocities are equalized. An interesting feature of the motion of the droplets in a flow, in which energy is released, may be observed by comparing the graphs of the velocities \overline{w} and \overline{u} in Figs. 1 and 2 for $10-\mu$ droplets. Although the mean size of the droplet in the reaction zone is less for disintegration than for evaporation, it is more slowly accelerated. This is because in the case of the disintegration model more energy is liberated over a given distance from the front than in the case of the evaporation model. Consequently, at a given x the value of \overline{u} is greater and that of $\overline{w} - \overline{u}$ less for disintegration, i.e., in this case the aerodynamic drag force acting on the droplet is less than for evaporation.

The width of the heat release zone for the evaporation model at droplet radii of 100 and 1000 μ is very great, and it may be assumed that in this case the energy losses to the walls will be so high that the steady-state propagation of detonation will be impossible.

The calculations for droplets more than 10 μ in size ended at degrees of combustion $1 - \sigma w \neq 1$; however, in the case of the disintegration model the extent of the heat release zone evidently does not much exceed the distance at which the computations were interrupted, since the subsequent breakup of the droplet and the high gas temperature lead to a considerable acceleration of the fuel reaction process.



Fig. 1. Variation of the parameters of the two-phase flow along the length of the heterogeneous detonation reaction zone (evaporation model). Droplet radius, μ : a) 10; b) 100; c) 1000.



Fig. 2. Variation of the parameters of the two-phase flow along the length of the heterogeneous detonation reaction zone (disintegration model in accordance with Eq. (9)). Droplet radius, μ : a) 10; b) 100; c) 1000.



Fig. 3. Variation of the parameters of the two-phase flow along the length of the heterogeneous detonation reaction zone (disintegration model in accordance with Eq. (10)). Droplet radius, μ : a) 10; b) 100; c) 1000.

Unfortunately, we lack experimental data on the lengths of the reaction zones in detonation waves in sprays. It is only possible to estimate them approximately from the data of [4]: for $r_0 = 140 \ \mu$, $x \approx 40 \ mm$ (estimated from a photographic time record of the detonation process), which is in good agreement with the calculated data; for $r_0 = 1.45 \ mm$, $x \approx 300 \ m$ (estimated from a shadowgraph of the wave). As for the evaporation model, the zone length for droplet disintegration increases considerably on transition to sprays

with larger droplets. A comparison of the burnup curves for both models shows that the rates of droplet combustion for the evaporation and disintegration mechanisms are comparable only for the finest droplets with $r_0 = 10 \mu$.

For a sufficiently slow variation of the degree of combustion (droplet radii of 100 and 1000 μ) the pressure behind the wave at first increases, approaches a maximum, and then falls. The final pressure, i.e., the pressure at the Chapman-Jouguet point, is always higher than in a gas detonation. The pressure rise at the beginning of the reaction zone is associated with the deceleration of the gas flow by the droplets.

The variation of the liquid-phase concentration σ behind the detonation front is represented in Figs. 3a, b. Only at high burning rates (Fig. 3,a) does $\overline{\sigma}$ fall directly behind the front. The increase in the liquidphase concentration behind the front is related with the change in droplet velocity. An increase in $\overline{\sigma}$ does not lead to enrichment of the mixture with the fuel component; on the contrary, the relative concentration $\sigma/\rho O_2$, where ρO_2 is the variable oxygen concentration, divided by the stoichiometric value of the component ratio \varkappa_0 ,

$$a = \frac{\overline{\sigma}}{\left(\frac{\rho_1}{\rho_0} \frac{1}{a_0^*}\right)\overline{\rho} - \frac{1}{\overline{u}}\left(1 - \overline{\sigma} \ \overline{w}\right)\left(1 + z_0\right)}$$

 $(\alpha_{0*}$ is the initial value of the ratio), behind the front always remains less than in the starting mixture. The greater leanness of the mixture is attributable to the increased density of the gaseous oxidizer, the initial value $\alpha = \alpha_0^*$ is actually restored when the gas and droplet velocities are equalized.

The kinetic energy of the droplets in the laboratory system, i.e., the energy expended on accelerating the droplets, is only 3-5% of the heat release behind the wave for the cases considered; accordingly, in the energy conservation equation we can neglect terms representing the kinetic energy of the droplets.

Although it was stated above that at We < We_{cr} the droplets break up into finer droplets and the heat release zone is evidently not much greater than the distances at which the calculations were interrupted, the question of the possible incomplete combustion of part of the fuel remains, since the fine droplets formed as a result of breakup are at rest relative to the gas and their burnup rate will be small. In the presence of a long droplet burnup zone the energy losses to the walls may lead to the expansion wave, whose head in the present calculations is determined by the condition $\overline{\sigma} = 0$, moving upstream to a point where $\overline{\sigma} \neq 0$. Droplets that react behind the head of the expansion wave cannot contribute to the energy of the shock wave; therefore the detonation wave will be propagated at a lower velocity than follows from the thermodynamic calculations (even if the direct energy losses to the walls are taken into account).

Thus, our calculations based on two different vaporization mechanisms have shown that:

1) breakup of the droplets considerably intensifies the combustion of the liquid as compared with the evaporation process;

2) the detonation model based on the assumption that the burning rate of the two-phase mixture is determined by the breakup rate evidently gives the correct value of the length of the reaction zone;

3) in the case of heterogeneous detonation the length of the reaction zone decreases sharply with decrease in the mean size of the liquid droplets;

4) the fraction of the energy released in the reaction zone expended on accelerating the droplets is small;

5) a complete calculation of the heterogeneous detonation reaction zone for sprays with droplet dimensions $r_0 \ge 100 \ \mu$ should take into account the deformation and disintegration of the droplets.

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