DEFORMATION OF DROPS IN THE REACTION ZONE OF HETEROGENEOUS DETONATION

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The development of theoretical ideas about heterogeneous detonation of combustible mixtures consisting of liquid fuel drops and a gaseous oxidizer is still a long way from the level of similar work in the field of gas detonation. Williams [1, 2] is evidently the first to investigate the structure of the reaction zone in a detonation wave propagating in a two-phase mixture. The works [1] and [2] prove the applicability of the Zel'dovich–Neiman–Dering model for heterogeneous detonation. Moreover, it is also noted in these works that the evaporation of the liquid phase cannot be the process which determines the rate at which the fuel is burned in heterogeneous detonation.

Since it is shown that the evaporation of drops behind the front of the detonation wave is negligible and makes only a small contribution to the overall heat emission, it is possible to analyze the influence of the disintegration and deformation processes of the drops of liquid on the extent of the reaction zone in heterogeneous detonation.

1. Presentation of the Problem. It is supposed that a linear plane detonation wave with a speed D is propagated in a two-phase medium which consists of a gaseous oxidizer and uniformly distributed drops of a liquid combustible fuel. The speed, pressure, density, and temperature of the gas before the front of the wave are u_0, p_0, ρ_0, and T_0, respectively; and at any point after the front they are u, p, ρ, and T. The state of the liquid phase before the detonation wave is characterized by the speed of the drops w_0, the dimensions of the drops r_0, and the mass concentration of liquid in a unit volume of gas σ_0. The magnitude σ_0 is determined by the ratio $\sigma_0 = 1.33\pi r_0^3 n_0 d$ (n_0 is the number of drops in a unit of volume, and d is the density of the liquid). The state of the liquid behind the detonation front is described by the speed of the drops w, the volume of an individual drop V, and the concentration of liquid which is given as $\sigma = Vnd$ in this region in view of the nonsphericity of the drops. The movement of a two-phase mixture is examined in a system of coordinates associated with the front of the wave, as a result of which $D = u_0 = w_0$. We will examine the basic simplifying hypotheses.

The hypotheses of [1] and [2] are usually used in analysis of two-phase flows and detonation waves.

1. The structure of the detonation wave corresponds with the Zel'dovich–Neiman–Dering hypothesis about a self-supporting steady impact wave with a subsequent deflagration zone.

2. The volume occupied by the drops of liquid is negligibly small in comparison with the volume of gas.

3. The influence of viscosity and thermal conductivity are effective only in the interaction processes of phases.

4. The drops of liquid do not combine and they do not oscillate with one another.

5. The drops are of equal size on the upstream side of the detonation front.

6. The temperature of the drops is constant, and the relationship between the surface tension of the liquid and the temperature variation of the viscosity of the gas is not taken into account.

On the basis of tests described in [4, 5] it is possible to come to the conclusion that the drops blown out by a high-speed flow of gas, $u - w > 20$ m/sec, assume a form which is similar to the shape of

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an ellipsoid of rotation. The minor axis of the ellipsoid, which is the axis of rotation, is oriented along the gas flow. Ranger and Nicholls [6] showed that the deformation of the drops into the ellipsoid of rotation is observed up to Weber and Reynolds numbers $W = 10^5$ and $R = 10^6$.

It is known from experiments on the disintegration of the drops that, after drops of a determined degree of deformation (which we will call critical) have been obtained, a rapid disintegration of the drop into a large number of finer drops is observed [3, 6]. The drop retains its integrity right up to the very moment that the critical stage of deformation is reached.

We will formulate the following basic hypotheses about the deformation of drops behind the front of the detonation wave:

1) The drops of liquid are deformed into the form of an ellipsoid of rotation, whose minor axes are parallel to the direction of the gas flow.

2) The critical stage of deformation is reached when the relationship between the length of the major semiaxis of the ellipsoid of rotation a and the initial radius of the drop is $a/r_0 = 3$ [6].

3) Right up to the moment of time while $a/r_0 \leq 3$, the disintegration of the drops takes place by the mechanism of the liquid drop [3, 6].

4) Until the moment at which the drops reach a critical stage of deformation, the model of a heterogeneous detonation remains correct; according to this model the disintegration of the drops according to the mechanism of collapse of the surface layer of liquid is considered to be a process which determines the rate at which the liquid phase burns out. In other words the rate of evaporation of the microdrops torn off from the initial drops and the rate of the mixing and the chemical reactions are considered to be high in comparison with the rate of the disintegration process.

2. Basic Equations. The equation of continuity for the two-phase mixture will be written as follows:

$$\rho_0 u_0 + \sigma_0 w_0 = \rho u + \sigma w \tag{2.1}$$

The equation of conservation of momentum has the form

$$\rho_0 u_0^2 + \sigma_0 w_0^2 + p_0 = \rho u^2 + \sigma w^2 + p \tag{2.2}$$

The equation of conservation of energy is written in the form

$$\rho_0 u_0 \left[\frac{\gamma_0 p_0}{(\gamma_0 - 1)\rho_0} + \frac{u_0^2}{2}\right] + \sigma_0 w_0 \left[cT_0 + Q + \frac{w_0^2}{2}\right] = \rho u \left[\frac{\gamma p}{(\gamma - 1)\rho} + \frac{u^2}{2}\right] + \sigma w \left[cT_0 + Q + \frac{w^2}{2}\right] \tag{2.3}$$

Here $\gamma = c_p/c_v$ is the ratio of the specific heats at constant pressure c_p and at constant volume c_v, c is the thermal capacity of the liquid, and T_0 is the temperature of the drops.

The equation of state of the gaseous medium

$$Mp = \rho T R^* \tag{2.4}$$

and the equation for conservation of total number of drops

$$nw = \text{const} \tag{2.5}$$

are added to these equations.

Here M is the molecular weight of the gas, R* is the gas constant, and T is the temperature of the gas.

If the major semiaxis of the ellipsoid has the dimension a, then the equation of movement of the drop will be

$$w\frac{dw}{dx} = -\frac{k\rho}{2Vd}(w - u)^2 \pi a^2 \tag{2.6}$$

Here x is the distance from the impact front, $k = 0.27R^{0.20}$ is the coefficient of resistance [7], $R = 2a(w - u)\nu^{-1}$, and ν is the kinematic viscosity of the gas.

The equation representing reduction in the volume of the drop on account of the collapse of the surface layer of the liquid drop will be written, in accordance with [3], as

$$w\frac{dv}{dx} = -4\pi\left(\frac{\nu}{\nu_f}\right)^{0.16}\left(\frac{\rho}{d}\right)^{0.33}\nu_f^{0.5}(w-u)^{0.5}a^{1.5} \tag{2.7}$$

Here ν_f is the kinematic viscosity of the liquid.

Theoretical concepts about the deformation of drops are examined in the works [3] and [8].

By converting the equation of deformation of the drop, obtained in [8], to a convenient form and neglecting the influence of surface tension and viscosity, we will obtain

$$Vd\frac{d^2s}{dt^2} = 0.5\pi a^2\rho(w-u)^2 \tag{2.8}$$

Here s is the displacement of the surface of the drop along the minor axis of the ellipsoid, and t is the time.

By changing over from the variable t to the variable z, we obtain

$$w^2\frac{d^2s}{dx^2} = 0.5\pi a^2(Vd)^{-1}\rho\left(k\frac{ds}{dx}+1\right)(w-u)^2 \tag{2.9}$$

The volume of the ellipsoid of rotation is given by $V = {}^4/_3\pi ba^2$, and therefore it remains to find the magnitude of the minor semiaxis b in order to establish the solution.

In the case of a constant mass of the drop $b = r_0 - s$. Taking into account the variation of the mass, we obtain

$$b = r(1 - sr_0^{-1}) \tag{2.10}$$

Here $r = 0.62V^{0.33}$ is the instantaneous value of the radius of the drop if it has remained spherical in the disintegration process.

Having defined the values of all the variables directly behind the impact front which leads to the detonation with the index 1, we change over to the dimensionless variables

$$w' = \frac{w}{w_0}, \quad u' = \frac{u}{u_0}, \quad \sigma' = \frac{\sigma}{\sigma_0}, \quad s' = \frac{s}{r_0}$$
$$\delta' = \frac{V^{0.33}}{r_0}, \quad n' = \frac{n}{n_0}, \quad x' = \frac{x}{r_0}, \quad p' = \frac{p}{p_1}$$
$$T' = \frac{T}{T_1}, \quad \rho' = \frac{\rho}{\rho_1}, \quad t' = \frac{tw_0}{r_0}, \quad M' = \frac{M}{M_1}$$

Omitting the indices here and in the future in the dimensionless parameters, we obtain the following form of Eqs. (2.1) and (2.2)

$$\rho u = AB, \quad pp_1 = 1 + \rho_0 u_0^2 p_0^{-1}(C - A\rho^{-1}B^2) \tag{2.11}$$

Here

$$A = \rho_0\rho_1^{-1}, \quad B = 1 + \sigma_0\rho_0^{-1}(1-\sigma w), \quad C = 1 + \sigma_0\rho_0^{-1}(1-\sigma w^2)$$

Making use of Eqs. (2.11) and (2.3), we present the dimensionless density of the gas in the form

$$\rho = ABDE^{-1}[1 + (1 - BED_1^{-2})^{0.5}] \tag{2.12}$$

Here

$$D = [p_0(\rho_0 u_0^2)^{-1} + C]\gamma(\gamma-1)^{-1}, \quad D_1 = D(\gamma-1)^{0.5}(\gamma+1)^{-0.5}$$
$$E = \frac{2\gamma_0 p_0}{(\gamma_0-1)\rho_0 u_0^2} + 1 + \sigma_0\rho_0^{-1}\left[\frac{2(cT_0+Q)}{u_0^2}(1-\sigma w) + 1 - \sigma w^3\right]$$

Equation (2.12) can be simplified if we pay attention to the fact that in the detonation wave $p_0/\rho_0 u_0^2 \ll 1$, and in the Chapman–Zhuge plane $\sigma = 0$, and $1 - BED_1^{-2} = 0$.

The dimensionless form of the equations of the state and of the conservation of the total number of drops is as follows:

$$Mp = \rho T, \quad F\sigma w = \delta^3 \tag{2.13}$$

in which $F = 4/3\pi$, $M \approx 1$.

The equations of movement and loss in the volume of the drops have the dimensionless form

$$w\frac{dw}{dx} = -A_1(w-u)^{2.21}(\sigma w)^{-0.26}\rho(1-s)^{-1.1} \tag{2.14}$$

$$w\frac{d(w\sigma)}{dx} = -A_2(w-u)^{0.5}\rho^{0.33}(\sigma w)^{0.5}(1-s)^{-0.75} \tag{2.15}$$

After introducing an additional variable $ds/dx = \eta$ we obtain an equation for deformation of the drops

$$w\frac{d\eta}{dx} = A_1\frac{(w-u)^{2.21}\rho\eta}{(\sigma w)^{0.26}(1-s)^{1.1}} + A_3\frac{\rho(w-u)^2(\sigma w)^{0.33}}{(1-s)} \tag{2.16}$$

The coefficients A_1, A_2, A_3 are determined by the relationships

$$A_1 = 0.1\rho_1 \quad d^{-1}R_0^{0.21}, \quad A_2 = 4.2(\nu_f\nu^{-1})^{0.33}(\rho_1 d^{-1})^{0.33}R_0^{-0.5}$$

$$A_3 = 0.375\rho_1 d^{-1}, \quad R_0 = w_0 r_0 \nu_0^{-1}$$

In order to obtain a fuller picture of the process, the same equations were written in the coordinates of the time t with the origin on the front of the detonation wave. These equations can be derived from those written above:

$$\begin{aligned} \frac{dw}{dt} &= -A_1(w-u)^{2.21}\rho(\sigma w)^{-0.33}(1-s)^{-1.1} \\ \frac{d(\sigma w)}{dt} &= -A_2\rho^{0.33}(w-u)^{0.5}(\sigma w)^{0.5}(1-s)^{-0.75} \\ \frac{ds}{dt} &= \varphi, \quad \frac{d\varphi}{dt} = A_3\rho(w-u)^2(\sigma w)^{-0.33}(1-s)^{-1} \end{aligned} \tag{2.17}$$

3. Calculation and Discussion of Results. Solution of the system of equations (2.14)-(2.16) and (2.17) was achieved numerically by the method of finite differences on the electronic digital computer "Mir-1." The calculation was carried out for a two-phase mixture, which consisted of drops of heptane and gaseous oxygen. The thermodynamic calculated value of the rate of detonation, for a stoichiometric composition of this mixture ($\sigma_0/\rho_0 = 0.284$) and when the initial pressure and temperature of the mixture $p_0 = 1$ atm and $T_0 = 300°K$, is D = 2400 m/sec [9]. Two variants of a monodisperse dispersion of heptane in oxygen with drop dimensions of $r_0 = 0.1$ mm and $r_0 = 1$ mm are examined. A characteristic of the computation is the examination of the magnitude of the relative deformation s of the liquid drop. It follows from Eq. (2.9) that in the case of $a/r_0 = 3$ the value of the critical stage of deformation is $s^* = 0.9$. On this basis the computations were terminated at $s = s^* = 0.9$.

The results of numerical calculation of the parameters of a two-phase flow behind the front of a detonation wave are given in Fig. 1. It is seen from the graph that reaching of the critical shape of deformation of the drops of liquid, that is, s = 0.9, takes place at the moment when, on account of the collapse of the surface of liquid, the original mass of the drop is successfully reduced by $(1 - \sigma w) \approx 0.08$ in drops whose radius is $r_0 = 10^2\mu$ (Fig. 1a) and only by $(1 - \sigma w) \approx 0.02$ in drops with $r_0 = 10^3\mu$ (Fig. 1b). At the moment of of time when $s = s^* = 0.9$ the relative speed of the gas and the drops is high and it is about 10^3 m/sec. The absence of experimental data about the spectrum of the dimensions of the drops which form when the original drops break up prevents us, for the present, from finding by computation the time interval and distance necessary for them to evaporate, mix, and burn up. However, if we take the dimensions of the newly formed microdrops in a rough approximation equal to 2b (where $s = s^* = 0.9$), it is possible to show that the completion of drops with a dimension of $r_0 = 10^2\ \mu$ is completed on account of the evaporation at a distance $x \approx 10$ mm from the detonation front, but that of drops with a dimension of $r_0 = 10^3\mu$ is completed at a distance of x = 100 mm. According to the evaporation model [1], the length of the reaction zone for drops with $r_0 = 10^2\ \mu$ was $x \approx 1$ m, and for drops with $r_0 = 10^3\mu$ it was $x \approx 6$ m. According to the disintegration model and according to the mechanism of the surface layer of the liquid drops, the same values are obtained, respectively, $x \approx 60$-100 mm ($r_0 = 10^2\mu$) and $x \approx 0.6 - 1$m ($r_0 = 10^3\mu$). Hence, the deformation of the drops in the reaction zone, which facilitates rapid destruction of the drops, obviously leads to the lowest values for the length of the reaction zone.

In the case of heterogeneous detonation in mixtures with drops whose dimensions are $r_0 = 0.1$ mm the critical stage of deformation, that is, $s = s^* = 0.9$, is reached $1 \cdot 10^{-6}$ sec after contact of the drops with the

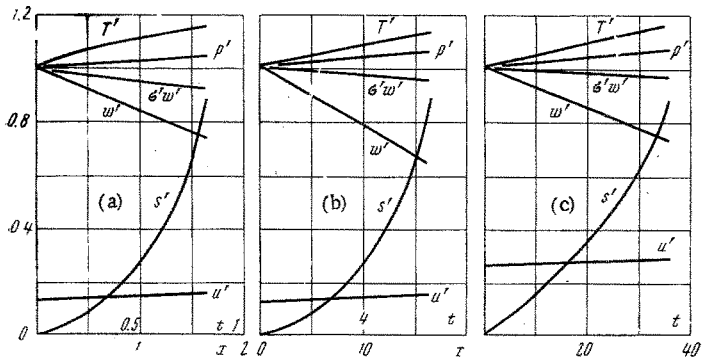

Fig. 1

front of the wave. Hence, obviously the formation of a homogeneous gas mixture behind the front of the wave takes place after times which are close in order of magnitude to the period of induction of combustion of gaseous mixtures of such composition, after they have been compressed at the front of the detonation wave. The detonation speed in such a heterogeneous mixture will not differ from the speed of detonation in a homogeneous gas mixture of equivalent composition, since the energy losses from the reaction zone will be practically the same. For mixtures of stoichiometric composition the experimental values of the speed of detonation will differ little from the calculated value. Data which confirm the agreement of calculated magnitudes of the speeds of detonation with experimental measurements are obtained in [9] from measurement of the detonation speed in combustible aerosols with drop dimensions $r_0 \leq 0.8$ mm.

The propagation of the detonation in two-phase mixtures with drops $r_0 \geq 1$ mm requires special examination. It is easily seen from the graphs of Fig. 1 that as the dimensions of the drops increase, the length of time which is necessary in order that $s = s^*$ increases considerably. Evidently this circumstance together with a number of others given below leads to the fact that the magnitude of the speed of detonation in a similar two-phase mixture, as the authors of [9] and [10] have shown, drops to values which are only about 50% of the calculated value. Similar detonation conditions are unknown in homogeneous gas mixtures. A disintegration of the detonation wave is observed even in the case of small decrease in the speed of the gas detonation (by 10-15%). In order to explain the mixture of detonation waves in heterogeneous mixtures with large drops, a calculation was made of the change in the parameters of a two-phase heptane–oxygen mixture of stoichiometric composition with drops $r_0 = 1.3$ mm behind a detonation wave whose speed is $D = 1200$ m/sec. The results of the calculation are given in Fig. 1c. The critical stage of deformation $s = s^* = 0.9$ is reached after a time $t \approx 3.5 \cdot 10^{-5}$ sec. After this time only 2% of the original mass ($1 - \sigma w = 0.02$) was successfully broken away as a result of stripping of the surface layer of liquid from the drop. We will compare the calculated data which we have obtained with the experimental results given in [10] in which a series of photographs are given which represent the transformations undergone by the drop of liquid $r_0 = 1.3$ mm behind the front of the wave when $D = 1200$ m/sec. The deformation of the drop and the breaking away of the secondary microdrops become noticeable already after a time interval of $t = (3\text{-}6) \cdot 10^{-6}$ sec and progress with time. The deformation of the drop is manifested in the increase of the dimensions of its lateral cross section which is parallel to the plane of the front of the wave.

However, right up to $t \approx 40 \cdot 10^{-6}$ sec the photographs of the disintegrating drop in a neutral [6] and oxidizing [10] medium are similar to each other, which evidently confirms the unimportant influence of combustion on the development of the process at this stage. In accordance with the model developed in Part 2 and with the known data about the disintegration of the drops [3-6], intensive disintegration of the drop begins after a time interval of $t = t(s^*) \approx 35 \cdot 10^{-6}$ sec after contact of the front of the wave with the drop. The authors [10] observed a strong secondary explosion in the depth of the zone behind the forward face of the front. In all likelihood the cause of secondary detonation is the formation, as a result of an intense initial disintegration of the drop, of local sources of combustible mixture and their very high rate of combustion, which serves as an excitation source for secondary impact waves. The secondary impact waves, which form as a result of combustion of the sources of the explosive mixture, overtake the front of the initial wave and carry out transmission of energy from the zone of the main heat generation to the impact wave.

The secondary waves, retreating in the opposite direction, transfer part of the energy into the detonation products. The main energy losses are, however, associated with a time delay of the process of final burning of the disintegrated drop. After the drop has disintegrated, the energy emission process is limited by the rate of the mixing process of the components of the mixture, which, judging from the results of [6], continues for a time period $t = 6r_0(v_1 - w_1)^{-1} (\rho_1^{-1}d)^{0.5}$. It is necessary to anticipate that the substantial part of the energy liberated at this stage does not contribute to maintenance of the detonation wave since because of the great length of the reaction zone the losses of energy to the tube wall are high, and the liberation of energy can take place already after the "head" of the rarefaction wave.

Hence, in the case of fine-drop spray detonation the heat emission process takes place in a quasi-homogeneous manner (almost as in the case of gaseous detonation). The extent of the zone of heat emission is hence comparable with the length of the same zone in the case of gaseous detonation. As a result of the above-mentioned circumstances the magnitude of the speed of the waves of a heterogeneous detonation, as well as of the waves of a gaseous detonation, differs negligibly from the value calculated by the thermodynamic theory of gases.

Considerable increase in the diameters of the drops leads to nonuniformity of the distribution of the fuel concentration in the volume behind the front of the wave and to occurrence of intensive secondary impact waves and of clearly expressed nonuniformity of the heat emission process (and also, evidently, to incomplete burning). As a result of substantial energy losses from the reaction zone, the detonation speed in mixtures with large drops must be less than the calculated speed.

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