

HYDROGASDYNAMICS IN TECHNOLOGICAL PROCESSES

EXCITATION OF SHOCK WAVES IN THE PASSAGE OF DETONATION THROUGH THE REGION OF MIXING OF REACTING AND INERT GASES

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A nonstationary problem on the excitation of a plane shock wave as a result of the passage of detonation through the region of mixing of a reacting and an inert gases has been formulated and solved numerically. The formulation of this problem is based on the approximate model defining, with a high accuracy, the change in the molar mass and specific internal energy of the combustion products of hydrocarbons caused by a shift of them from their chemical-equilibrium position. A situation in which, in the region of mixing of the reacting and inert gases, their concentrations change linearly was considered. The influence of the width of the mixing region on the intensity of the excited shock waves and the law of their attenuation was investigated.

Keywords: gas detonation, reacting and inert gases, detonation products, chemical equilibrium, shock wave.

Introduction. If any space is filled partially with a reacting gas or, more precisely, a combustible gas mixture, and the remainder of this space is occupied by an inert gas, e.g., by air, a detonation of the reacting gas will give rise to a shock wave in the inert gas. The excitation of shock waves by a gas detonation is of interest in connection with the problems of explosion safety as well as to the development and modernization of different technological facilities in which detonation-combustion products are used as an actuating medium. Such facilities find application in engineering for the propulsion in engines and the force (destructive) action on objects, the intensification of combustion of a fuel, and the acceleration and heating of condensed particles [1–3].

Laws of attenuation, in air, of plane shock waves arising as a result of the formation of a Chapman–Jouguet wave in the explosion of a reacting gas [4] were investigated numerically in [5, 6]. A Chapman–Jouguet detonation wave with an instantaneous chemical reaction at its front is characterized by that the front of this wave moves with a constant velocity D_{CJ} and, in the case where such a wave propagates from a rigid wall and the motion of the detonation products is one-dimensional, it can be defined by a self-similar solution [7]. Note that the velocity of the Chapman–Jouguet wave front D_{CJ} is the most important and significant characteristic of any explosive, including gaseous ones. In [8], the problem on the excitation of shock waves by an overcompressed gas detonation formed as a result of the passage of a Chapman–Jouguet detonation wave from a wide pipe through a reducer to a narrow pipe was considered, and the overcompressed gas detonation was calculated by the algorithm proposed in [9]. It was shown that shock waves excited by an overcompressed gas detonation can have a higher intensity compared to the intensity of the shock waves excited by a Chapman–Jouguet detonation because the velocity of propagation of the front of an overcompressed gas detonation D as well as the pressure and dynamic head of the combustion products formed as a result of this detonation are larger than those in the case of Chapman–Jouguet detonation [10]. The main characteristic of the overcompressed gas detonation waves is the degree of their overcompression $\alpha = D/D_{CJ}$ ($\alpha \geq 1$).

In the mathematical formulation of the problems considered in [5, 6, 8], the possible mixing of a reacting and an inert gases was disregarded, i.e., it was assumed that, at the contact boundary between them, their concentrations and, consequently, the thermodynamic properties of the gaseous medium change abruptly. Because of this, the initial parameters of the nonstationary shock wave formed as a result of the refraction of a detonation wave at the contact boundary between the indicated gases were determined from the solution of the problem on the breakdown of an arbitrary gasdynamic discontinuity between the detonation products and the undisturbed inert gas [11, 12]. Thus, it was always assumed that a detonation wave is instantly transformed to a shock wave. This simplification in the simulation of the formation of a shock wave in a gaseous

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medium in a pipe is correct from the physical standpoint only in the case where a reacting and an inert gases in this medium are separated by a thin membrane which is removed at the instant a detonation is initiated. Such a situation was considered in [13] where numerical simulation of the indicated process was conducted in parallel with its experimental investigation. The calculation data on the change in the velocity of a shock wave, formed in an inert gas in a pipe with a membrane, depending on the distance between it and the membrane, were compared with the results of measurement of this velocity. This comparison has shown that the numerical solution is in fairly good qualitative and quantitative agreement with the experiment. Clearly these results cannot be extrapolated to the case where the region of mixing of a reacting and an inert gases in a pipe has finite sizes comparable with the sizes of the pipe. In this case, a detonation wave will propagate in the gaseous medium in the pipe during a definite period of time, which points to the fact that in the region of mixing of the reacting and inert gases there is a gradient of their concentrations and, therefore, the transformation of a detonation wave to a shock wave cannot be instantaneous. In our opinion, to define this process adequately, it is well to use the quasionedimensional approach to the simulation of the propagation of a detonation wave in a medium with a variable chemical composition, proposed in [14].

In the present work, the indicated approach has been further developed and applied to the substantiation of the behavior of both detonation and shock waves in a gaseous medium. With it the problem on the excitation of a shock wave by a gas detonation in the case where the concentrations of a reacting and an inert gases in the region of their mixing change linearly was solved numerically, i.e., the result of the partial diffusion mixing of these gases was simulated.

On the Analogy between the Behavior of Detonation and Shock Waves. The passage of detonation through the region of mixing of two reacting gases with a gradient of their concentrations was investigated numerically in [14]. It was established that, if the parameters of the detonation products downstream of a Chapman–Jouguet detonation wave in the first reacting gas are superior to the analogous parameters of the second reacting gas, as a result of the passage of detonation through the region of mixing of these gases, overcompressed gas detonation waves can be excited. In this case, the velocity of the front of an overcompressed detonation wave D can even decrease but it will exceed the local velocity of the Chapman–Jouguet detonation wave front D_{CJ} characteristic of the chemical composition of the medium in the indicated region of the space. This allows the preliminary conclusion that, in the region of mixing of a reacting and an inert gases, a detonation wave should propagate in the overcompressed regime.

There is much in common between the overcompressed gas detonation waves with an instantaneous chemical reaction at their front, as a result of which an energy in the form of heat Q is released, and shock waves. In the case of this reaction, an equilibrium flow of detonation products is realized downstream of the detonation front. Overcompressed and shock waves are nonstationary as a rule, because the relative gas flow downstream of their front is subsonic. According to [15], the attenuation of these waves can be defined in one and the same context with the use of relations identical in their general form. If an inert gas contains polyatomic molecules, they downstream of the front of intense shock waves can dissociate into atoms with absorption of heat as does, e.g., oxygen in air, i.e., in a shock-compressed gas there can also take place chemical reactions that, unlike the reaction of transformation of a reacting gas to detonation products, are reversible. The thermal effect Q of the chemical reaction at the front of a shock wave is zero or negative. Because of this, the notion of inert gas is rather conditional. Detailed equilibrium calculations [16] have shown that the thermal effect Q at the detonation front is substantially dependent on the velocity of its movement D . For example, the Chapman–Jouguet detonation provides the largest Q . At $\alpha = 1.5–1.7$, the thermal effect decreases almost to zero and, as the velocity of movement of the detonation front further increases, Q becomes even negative. In this case, the differences between an overcompressed and a shock wave in a shock-compressed gas almost disappear if the thermodynamic properties of this gas are defined the model proposed in [17] and applied to the detonation product in [14].

Prior to the formulation of a concrete problem on the transformation of a detonation wave to a shock wave at the diffused boundary between a reacting and an inert gases, we make the following assumption. An attenuated overcompressed wave propagates in the Chapman–Jouguet detonation regime with a front velocity D_{CJ} , and, when a shock wave formed decays, it degenerates to an acoustic wave with a front moving with a velocity equal to the velocity of sound c_0 in an undisturbed medium. With this assumption it may be suggested that a weak shock wave is a detonation wave with a zero thermal effect at its front, and the velocity of sound c_0 can be used for it as an analog of the front velocity D_{CJ} . Since the intensity of a shock wave is determined by the Mach number of the relative gas flow upstream of the shock front $M = D/c_0$, for uniformity, the degree of overcompression of detonation waves will be calculated by the formula

$$\alpha = \frac{M}{M_{CJ}} = \frac{D/c_0}{D_{CJ}/c_0}. \quad (1)$$

When using this formula, it is necessary to remember that the sound velocities in a reacting and an inert gases are different in value.

Formulation of the Problem. The half of a space with a rigid wall, coincident with its symmetry plane, to the right of this wall is considered. The origin of the coordinate system used is coincident with the rigid wall, and the x axis is perpendicular to it. The indicated half-space in the initial state has a pressure p_0 and a temperature T_0 , and it is filled with immovable gases ($u_0 = 0$): a reacting gas A and an inert gas B. The reacting gas occupies the region $0 < x < l_A$ adjacent to the rigid wall, and the inert gas occupies the region $x > l_B$ ($l_B \geq l_A$). The gases A and B are mixed in the region $l_A \leq x \leq l_B$. Thus, the characteristic width of the mixing region is $\Delta l = l_B - l_A$.

As in [14], the chemical composition of the indicated gases is characterized by the concentrations of the atoms of oxygen \bar{n}_O , carbon \bar{n}_C ($\bar{n}_C \leq \bar{n}_O$), hydrogen \bar{n}_H , nitrogen \bar{n}_N , and other monoatomic inert gases Z (\bar{n}_Z) in them. However, calculations are performed more conveniently with the use of the relative concentrations of these atoms

$$n_{s1} = \bar{n}_{s1} / \sum_{s1} \bar{n}_{s1}, \quad (2)$$

where $s1 = \{C, H, O, N, Z\}$ and the subscript 1 points to the fact that a substance s is monoatomic. Clearly, when the chemical composition of a gaseous substance changes (with distance away from the rigid wall), not only n_{s1} but also other initial parameters of the gas, such as the molar mass μ_0 , the density ρ_0 , the specific (per unit mass) internal energy U_0 , and the sound velocity c_0 , become dependent on the coordinate x . A set of these initial parameters (at constant values of p_0 and T_0) is quite sufficient for calculating, with the use of the approximate model for analysis of equilibrium flows of chemically reactive gases [17], not only the local velocity of the Chapman–Jouguet detonation front D_{CJ} for any coordinate x but also the corresponding values of the pressure p_{CJ} , density ρ_{CJ} , mass flow rate u_{CJ} , molar mass μ_{CJ} , temperature T_{CJ} , and equilibrium sound velocity c_{CJ} of the combustion products at the detonation front with an error smaller than 1%. Therefore, we will assume that the dependence $D_{CJ} = D_{CJ}(x)$ is known.

The model [17] defining the equilibrium state of detonation products is based on the two relations. The first of them is the equation for the total internal energy of the combustion products

$$U = U_{th} + U_{ch} = U(\mu, T), \quad (3)$$

including, in addition to the thermodynamic part of the specific internal energy of the gas U_{th} , its potential chemical energy U_{ch} . The second relation is the equation for the shift of the gas from its chemical-equilibrium position

$$F(\mu, T, \rho) = \text{const}, \quad (4)$$

relating the molar mass μ , temperature T , and density ρ of the detonation products. Using the equation for the ideal-gas state $p/\rho = RT/\mu$ in combination with (4), we bring expression (3) to the form

$$U = U(p, \rho),$$

which makes it possible to determine the equilibrium velocity of sound in the gas from the relation

$$c^2 = (p/\rho^2 - U_\rho)/U_p, \quad U_p = (\partial U/\partial p)_\rho, \quad U_\rho = (\partial U/\partial \rho)_p. \quad (5)$$

This relation is easily obtained from the energy equation in the form used in the formulation of the first law of thermodynamics. Note that relations (3)–(5) can be also used for the definition of the thermodynamic properties of a gas compressed by a strong shock wave with dissociation of molecules downstream of its front. If the chemical reactions in such a gas are disregarded, instead of Eq. (4), the natural relation $\mu = \mu_0$ can be used.

In accordance with [17], to correctly define the thermal effect of a chemical reaction $Q = U_{0,ch} - U_{ch}(p, \rho)$ in a gaseous medium, it is necessary to coordinate the origins of calculating the specific internal energy of the gas U and its internal energy in the initial state $U_0 = U_{0,th} + U_{0,ch}$. Note that $U_0 \neq U(p, \rho)$ because of the irreversibility of the chemical reaction arising in a gaseous medium as a result of its detonation. In view of this representation of the physicochemical parameters of a chock-compressed gas and the products of its detonation, the transformation of a detonation wave in this gas to a shock wave can proceed in the following way. Let, at the instant of time $t = 0$, near the right wall there arises a self-sustained detonation wave propagating in the gas A with a constant velocity $(D_{CJ})_A$. In the region of mixing of the gases A and B, as a result of the change in the parameters of the gas mixture upstream of the detonation front, the front velocity becomes variable: $D = D(x)$.

It is assumed that the detonation wave can be a Chapman–Jouguet wave ($\alpha = 1$) or an overcompressed wave ($\alpha > 1$). The local degree of overcompression α of such a wave is determined from relation (1) with the use of the known dependence $D_{CJ} = D_{CJ}(x)$ considered above. When the wave front passes from the region of mixing of the gases A and B to the region occupied by only the gas B, the concentration of the gas A decreases to zero. This automatically leads to a decrease in the thermal effect Q to a minimum value characteristic of the gas B. As a result, the differences between the front of detonation and the shock front disappear. Since both these fronts represent surfaces of a strong gasdynamic discontinuity, propagating with one and the same velocity, their thermal effects are equal. Then only the gas B begins to pass through the detonation front to the region with detonation products and, in so doing, gradually forms a "plug" of the shock-compressed inert gas between the front and the detonation products. We can say that, beginning from this time on, a detonation wave is formed, and it propagates in the gas B. This wave decays with time because of the decrease in the piston action of the detonation products.

Thus, the character of a wave (detonation or shock) formed in a gaseous medium is determined by the type of the gas (reacting or inert) passing through its front. The gas in the region of mixing of the gases A and B also represents a chemically reactive medium but with smaller (compared to the gas A) values of the front velocity D_{CJ} and the thermal effect for the Chapman–Jouguet detonation regime, and $Q_{CJ} > 0$ in this case. Since the behaviors of detonation and shock waves are analogous, it may be assumed that $Q_{CJ} = 0$ for the gas B. In the subsequent discussion we will use the following terminology. As long as the coordinate of the front of a wave is smaller than l_B , it will be the front of a detonation wave, otherwise we will have the front of a shock wave. If no addition concretization is required, we will simply talk about the wave front.

The behavior of the continuous medium downstream of the wave front will be defined by the system of one-dimensional gasdynamic equations

$$\rho_t + (\rho u)_x = 0 ,$$

$$(\rho u)_t + (p + \rho u^2)_x = 0 , \quad (6)$$

$$[\rho(U + u^2/2)]_t + [\rho u(U + u^2/2 + p/\rho)]_x = 0 ,$$

to which it is necessary to add the equations for the change in the concentrations of atoms of the chemical elements in the process of movement of the medium (an analog of the continuity equation for the density of the medium)

$$(\bar{n}_{s1})_t + (\bar{n}_{s1}u)_x = 0 , \quad s1 = \{C, H, O, N, Z\} \quad (7)$$

with the following boundary conditions. At the left boundary of the computational region (at the rigid wall), the impermeability conditions are set (the mass velocity of the gas $u = 0$). At the moving right boundary of the computational region, the relations defining the laws of the mass, momentum, and energy conservation at the wave front

$$\rho(D - u) = \rho_0 D ,$$

$$p + \rho(D - u)^2 = p_0 + \rho_0 D^2 , \quad (8)$$

$$U(p, \rho) + p/\rho + (D - u)^2/2 = U_0 + p_0/\rho_0 + D^2/2$$

are true. At the right boundary of the computational region, relations (8) for a self-sustained detonation wave are supplemented by the Chapman–Jouguet condition for the equilibrium velocity of sound

$$D_{CJ} - u_{CJ} = c_{CJ} , \quad (9)$$

and these relations for a nonstationary overcompressed wave are supplemented by the relation for the characteristic c_+ at the wave front [9] following from the system of equations (6)

$$\frac{\partial u}{\partial t} + \frac{1}{\rho c} \frac{\partial p}{\partial t} + (u + c) \left(\frac{\partial u}{\partial x} + \frac{1}{\rho c} \frac{\partial p}{\partial x} \right) = 0 . \quad (10)$$

Therefore, the initial distribution of the parameters of detonation products can be represented in the form of a simple (Riemann) wave defined by the two ordinary differential equations and the ratio between the self-similar variable x/t , the mass velocity u , and the sound velocity c

$$dp = \rho c du, \quad d\rho = \rho/c du, \quad u + c = x/t, \quad (11)$$

on condition that the gasdynamic parameters of the detonation products at the detonation front correspond to the Chapman–Jouguet state. In order that this solution be valid, it is necessary that the chemical composition of the initial reacting gas be constant in the small neighborhood of the rigid wall. Since the initial pressure p_0 and temperature T_0 are independent of the coordinate x , the total concentration of the molecules $\bar{n} = \bar{n}_A + \bar{n}_B$ at all the points of the half-space $x > 0$ is constant:

$$\bar{n} = p_0/RT_0 = \text{const}. \quad (12)$$

It was assumed in the formulation of the problem that, in the region of mixing of the chemical substances, the concentrations of the gases A and B change linearly. Let us denote the mole fraction of the gas A in the gas mixture by $\varepsilon = \varepsilon(x)$, where $\varepsilon = 1$ at $x \leq l_A$ and $\varepsilon = 0$ at $x \geq l_B$. In this case, the initial parameters of the region of mixing of the gases A and B can be determined in view of (12) as

$$\begin{aligned} \mu_0 &= \varepsilon(\mu_0)_A + (1 - \varepsilon)(\mu_0)_B, \quad \rho_0 = \varepsilon(\rho_0)_A + (1 - \varepsilon)(\rho_0)_B, \\ U_0 &= [\varepsilon(\mu_0 U_0)_A + (1 - \varepsilon)(\mu_0 U_0)_B]/\mu_0(x), \\ \bar{n}_{s1}(x) &= \varepsilon(\bar{n}_{s1})_A + (1 - \varepsilon)(\bar{n}_{s1})_B, \quad s1 = \{C, H, O, N, Z\}, \end{aligned} \quad (13)$$

where $\varepsilon = (l_B - x)/\Delta l$ is a linear function of x , i.e., the concentration gradient of the chemical compound is inversely related to the width of the mixing region ($\sim 1/\Delta l$).

Results of Calculations. We used a stoichiometric mixture of acetylene with oxygen $C_2H_2 + 2.5O_2$ for the gas A and an air with a chemical composition $0.21O_2 + 0.78N_2 + 0.01Ar$ for the gas B. The gases A and B with an initial pressure $p_0 = 101,325$ Pa (1 atm) and an initial temperature $T_0 = 298.15$ K had the following parameters: $(\bar{n}_C)_A = 23.36$ mole/m³, $(\bar{n}_C)_B = 0$, $(\bar{n}_H)_A = 23.36$ mole/m³, $(\bar{n}_H)_B = 0$, $(\bar{n}_O)_A = 58.39$ mole/m³, $(\bar{n}_O)_B = 17.17$ mole/m³, $(\bar{n}_N)_A = 0$, $(\bar{n}_N)_B = 63.76$ mole/m³, $(\bar{n}_{Ar})_A = 0$, $(\bar{n}_{Ar})_B = 0.2861$ mole/m³, $(\mu_0)_A = 30.29$ g/mole, $(\mu_0)_B = 28.97$ g/mole, $(\rho_0)_A = 1.238$ kg/m³, $(\rho_0)_B = 1.184$ kg/m³, $(c_0)_A = 329.8$ m/s, $(c_0)_B = 346.1$ m/s, $(U_0)_A = -6.534$ MJ/kg, $(U_0)_B = -3.365$ MJ/kg.

Problem (1)–(3) was solved numerically by the method of breakdown of a gasdynamic discontinuity on moving meshes (by the Godunov scheme) [11] with separation of the right boundary (the wave front). Before a detonation wave reached the region of mixing of the gases A and B, the parameters of the gas mixture at the wave front were constant and corresponded to the parameters of the gas A in the case of Chapman–Jouguet detonation: $(D_{CJ})_A = 2424$ m/s, $(M_{CJ})_A = 7.350$, $(u_{CJ})_A = 1111$ m/s, $(c_{CJ})_A = 1313$ m/s, $(p_{CJ})_A = 33.91$ atm, $(\rho_{CJ})_A = 2.286$ kg/m³, $(\mu_{CJ})_A = 23.32$ g/mole, $(T_{CJ})_A = 4215$ K, and $(Q_{CJ})_A = 4.142$ MJ/kg. The distribution of the detonation products downstream of the front of the indicated detonation wave corresponded to the solution obtained in [14]. This distribution can be approximated analytically in the following way [18]:

$$\begin{aligned} \frac{u}{(u_{CJ})_A} &= \begin{cases} 2x/x_* - 1, & \text{at } 0.5 < x/x_* \leq 1 \\ 0, & \text{at } 0 \leq x/x_* \leq 0.5 \end{cases}, \\ \ln \frac{p}{(p_{CJ})_A} = \ln \frac{\rho}{(\rho_{CJ})_A} &= \begin{cases} 2x/x_* - 2, & \text{at } 0.5 < x/x_* \leq 1 \\ -1, & \text{at } 0 \leq x/x_* \leq 0.5 \end{cases}, \end{aligned}$$

where x_* is a coordinate of the wave front.

For increasing the accuracy of calculations by the above-described scheme, the velocity of the front of an overcompressed wave at the boundary of the computational region was determined not from the solution of the problem on the breakdown of a gasdynamic discontinuity but, as in [12], by the Riemann invariant for the characteristic c_+ at the wave front. We turned to the calculation of the wave-front velocity by relations (8) and (10) at the instant the following condition began to fulfill for the detonation products in the neighborhood of the wave front [9]:

$$u + c > D_{CJ},$$

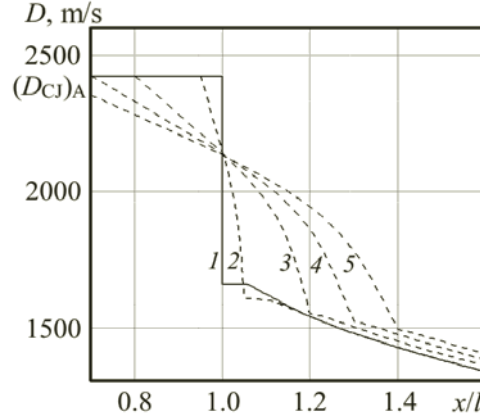


Fig. 1. Velocity of the wave front D depending on its position in the pipe, calculated for $\Delta l/l = 0$ (1), 0.1 (2), 0.4 (3), 0.6 (4), and 0.8 (5).

where D_{CJ} is a local velocity of the Chapman–Jouguet detonation front calculated in advance by relations (8) and (9), otherwise it was assumed that $D = D_{CJ}$.

Since the gases A and B have different values of the initial parameters ρ_0 and U_0 , in order that the mass and energy balance be retained in the system being considered in the case of change in Δl , it is necessary that the condition $l = (l_A - l_B)/2 = \text{const}$ be fulfilled. Therefore, before the initiation of detonation, the volume of the gas A in the half-space will be always constant. In this case, the increase in Δl can be interpreted from the practical standpoint as an increase in the width of the region of diffusion spreading of the boundary between the two contacting gases [19], and the coordinate of the left boundary of the region of mixing of these gases $l_A = l - \Delta l/2$ will be shifted to the rigid wall. Since $l_A \geq 0$ in the formulation of the problem being considered, the width of the mixing region is limited from above: $\Delta l \leq 2l$, where l is a characteristic spatial scale of the problem. Therefore, on condition that $\Delta l/l = \text{const}$, the dependences of all the parameters of the problem on the dimensionless coordinate x/l , calculated for different values of l , will be coincident. It follows herefrom that the solution of the problem in this formulation possesses a similarity and is determined by the single dimensionless parameter $\Delta l/l$. In view of (13), this parameter allows one to estimate the mass fraction of the gas A found in the mixing region before the initiation of detonation: $\delta = 0.5\Delta l/l \cdot 100\%$.

Figure 1 demonstrates the dynamics of change in the velocity of the front of a detonation wave D in the mixture of the gases A and B in a pipe in the process of its transformation into a shock wave at different values of the mixing region. Here, the results of calculations performed for the case where $\Delta l = 0$ and the wave front changes abruptly at the contact boundary between the reacting and inert gases are also presented. The abrupt change in the front velocity D (curve 1) from $(D_{CJ})_A$ to $\bar{D}_0 = 1658$ m/s was determined from the solution of the problem on the breakdown of a gasdynamic discontinuity. Note that \bar{D}_0 limits of the velocities of the shock waves excited in the case where the width of the mixing region is finite from above, i.e., this value of the front velocity is limiting. Curves 2–5 also have sharp inflections at the point $x = l_B$ ($l_B = l + \Delta l/2$) where the detonation front is transformed to the shock front. At this instant of time, the velocity of the shock front is maximum. We denote it by \bar{D} ($D \leq \bar{D}_0$). In this case, the coordinates of the inflection point of the curves in Fig. 1 can be defined as l_B/l , \bar{D} . To this point corresponds a shock wave propagating in the gas B with a Mach number $\bar{M} = \bar{D}/(c_0)_B$. We call the reader's attention to the similarity of the slopes of all the curves corresponding to the decay of the shock waves passing through the mixing zone. At $x > l_B$ the law of decreasing the velocity of the shock front can be approximated by the dependence

$$d(\ln D)/d(\ln x) = -1/2. \quad (14)$$

This result conforms with the conclusions of the point-explosion theory for adiabatic plane gas flows [20]. If we draw a line through the points of inflection of curves 2–5, this line will cross curve 1. A refinement of the results obtained has shown that this intersection takes place at $x/l = 1.15$ and corresponds to the calculated dependence $D = D(x/l)$ at $\Delta l/l = 0.3$. In accordance with (14), at $x/l > l_B/l = 1.15$, the graph of this dependence is almost coincident (with an accuracy as high as 1%) with curve 1. This statement is also true for the other curves $D = D(x/l)$ calculated for smaller values of $\Delta l/l$, even though their inflection points are positioned lower than curve 1. In this case, \bar{D} differs insignificantly from D_0 .

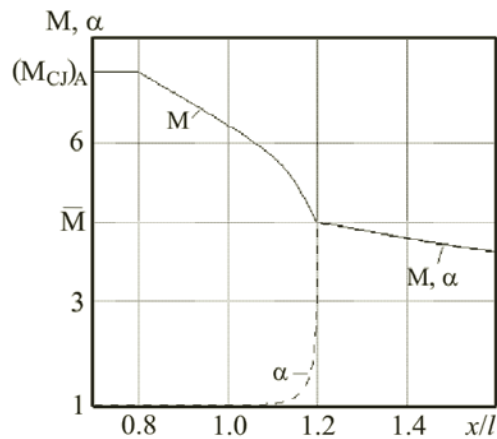


Fig. 2. Dependences of the Mach number M and the degree of overcompression α of a detonation wave on the dimensionless coordinate of the wave front x/l at a width of the mixing zone $\Delta/l = 0.4$.

For example, for curve 2, this difference comprises only 3%. It is seen that curve 2, as also curve 1, includes a small horizontal portion showing that the wave propagates with a constant velocity. This allows the conclusion important for practice that, only on the basis of experimental data on the velocity of the front of a shock wave in the region of a pipe $x/l > 1.15$, it is impossible to answer the question: Was the boundary between the reacting and inert gases diffused before the initiation of detonation at values of the ratio Δ/l as large as 0.3, which can be called a critical value? Thus, at $\Delta/l < 0.3$ ($\delta < 15\%$) the influence of the mixing of the gases on the dynamics of a shock wave excited in air can be disregarded. Another distinctive feature of the process being considered is the intersection of all the curves in the vicinity of one point with a dimensionless coordinate $x/l = 1$; in this case, the velocity of the wave front D in the region $l_A < x < l$ in the mixing zone changes almost linearly. This can be explained by the fact that, in the indicated region, the degree of overcompression of the wave α is almost equal to unity, i.e., the wave front moves with a velocity equal to the local velocity of the Chapman–Jouguet detonation front D_{CJ} . Note that, in accordance with (13), before the initiation of detonation in the gas mixture, its chemical composition and other parameters at the cross section of the pipe with a coordinate $x = l$ remain the same in all the cases considered in the calculations.

The dependence presented in Fig. 2 shows how the degree of overcompression α and the Mach number of a detonation wave change in the process of its passage through the mixing region. At $x/l = 1$, the velocity of the wave front exceeds D_{CJ} only by 2%, and $\alpha = 1.06$ at $x/l = 1.1$. The degree of overcompression of the wave begins to markedly respond to the change in the chemical composition of the gas only at the end of the mixing region where it reaches its maximum possible value $\alpha = \bar{M}$. For obviousness, a horizontal dotted line ($\bar{M} = 4.485$) is drawn through this point. The quantity \bar{M} is a minimum possible Mach number for the detonation front and, at the same time, a maximum Mach number for the shock front. In the case of propagation of a shock wave in the gas B, in accordance with (1), the values of M and α are equal. Therefore, the intensity of this wave can be characterized by only the parameter M , with which one can calculate all the other gasdynamic parameters of the mixture at the wave front [4].

The influence of the dimensionless width of the mixing zone Δ/l , representing the solution of the problem, on the Mach number \bar{M} can be estimated by the dependence presented in Fig. 3. It is seen that the maximum Mach number for a shock wave in the gas B is limited: $\bar{M}_2 < \bar{M} < \bar{M}_0$, where the value of $\bar{M}_0 = 4.791$ was determined from the solution of the problem on the breakdown of a gasdynamic discontinuity at $\Delta/l = 0$, and the value of $\bar{M}_2 = 3.973$ was determined, in view of condition (1), at $\Delta/l = 2$. It follows herefrom that, when the parameter Δ/l is varied, the intensity of the shock wave changes approximately by 20% ($\bar{M}_0/\bar{M}_2 = 1.206$). The curve in Fig. 3 approaches the point \bar{M}_0 on the y axis almost in touch. In the case where the width of the mixing zone is small ($\Delta/l \rightarrow 0$), it is necessary to use a difference mesh with small nodes. Therefore, a minimum value of the ratio Δ/l equal to 0.01 was used in the calculations of the mixing zone with a spatial resolution. At $\Delta/l = 0.01$, the maximum Mach number for a shock wave excited by a detonation in the inert gas differed from \bar{M}_0 by less than 1%. This tendency is also characteristic of the case where the chemical composition of the reacting gas is varied. In Fig. 4, the results of calculations, in which a methane–oxygen mixture $\text{CH}_4 + 2\text{O}_2$ was used for the gas A, are presented for comparison. In accident-related explosions, e.g., in mines, air can be an oxidizer.

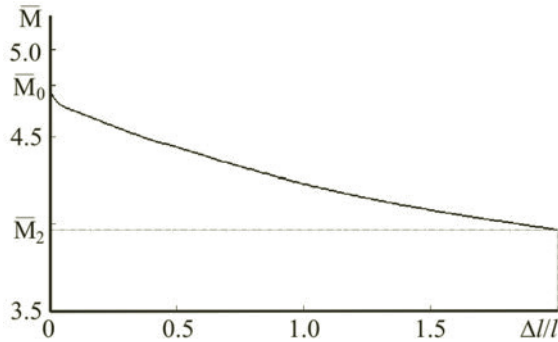


Fig. 3. Maximum Mach number \bar{M} for the shock wave excited by a detonation in the inert gas depending on the dimensionless parameter of the problem Δ/l .

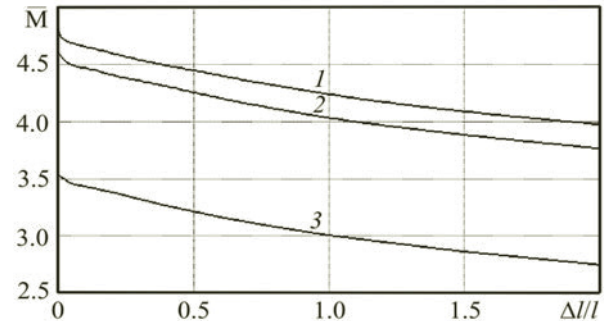


Fig. 4. Dependences $\bar{M} = \bar{M}(\Delta/l)$ calculated for the cases of excitation of shock waves in air by detonation of different gas mixtures: 1) $C_2H_2 + 2.5O_2$; 2) $CH_4 + 2O_2$; 3) stoichiometric mixture $CH_4 + \text{air}$.

Note that, in addition to the explosion-safety problems, the results obtained can be used for solving a number of applied problems, e.g., problems associated with detonation spraying. The point is that modern detonation facilities can work in the case where their channel is partially filled with an explosive and the rest is filled with an inert gas or air. In this case, a powder for deposition is introduced as a rule into the region of contact of the reacting and inert gases [3]. Therefore, the more accurate is the definition of the gas dynamics of the flow in the region of mixing of the reacting and inert gases, the more accurate will be the calculation of the velocity and temperature of the particles to be thrown determining the quality of the detonation coating.

Conclusions. Computational experiments simulating the transformation of a detonation wave to a shock wave at a diffused contact boundary between a reacting gas (a stoichiometric mixture of acetylene with oxygen) and an inert gas (air) have been conducted. The influence of the width of the region of mixing of the contacting gases on the intensity of the shock waves excited in it and on the law of their attenuation was investigated. The solution obtained possesses a similarity and is determined by a single parameter (the dimensionless width of the mixing region) which, in fact, is equivalent to the mass fraction of the reacting gas that has managed to mix with the inert gas before the initiation of detonation. When this parameter is varied within the range from 0 to 2, the maximum Mach number of a shock wave in the inert gas decreases by approximately 20%. It was established that the law of decreasing the velocity of the wave front can be approximately defined by the dependence corresponding to the conclusions of the point-explosion theory for adiabatic plane waves.

NOTATION

c , velocity of sound, m/s; D , velocity of the detonation front, m/s; l , coordinate of the contact boundary between the gases, m; Δl , width of the mixing region, m; M , Mach number; \bar{n} , concentration of atoms, mole/m³; n , relative concentration of atoms; p , pressure, atm; Q , thermal effect of a chemical reaction, J/kg; R , gas constant, J/(mole·K); t , time, s; T , temperature, K; u , mass velocity, m/s; U , specific internal energy of a gas (per unit mass), J/kg; U_{th} , thermodynamic part of the internal energy of a gas, J/kg; U_{ch} , potential chemical energy of a gas, J/kg; x , current coordinate, m; x_* , coordinate of the front of a detonation wave, m; α , degree of overcompression of a wave; μ , molar mass, kg/mole; ρ , density, kg/m³. Subscripts: CJ, indication of the Chapman–Jouguet state; ch, chemical; th, thermodynamic; 0, value of a gasdynamic parameters of the mixture in the initial state upstream of the wave front.

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