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Determination of the Velocity of the Detonation Wave and the Conditions for the Appearance of Spherical Detonation during the Interaction of Hydrogen with Oxygen

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Abstract

The well-known formula for the flat detonation wave velocity derived from the Hugoniot system of equations faces difficulties, if being applied to a spherical reactor. A similar formula has been obtained in the framework of the theory of explosion in reacting gas media with the use of a special model describing the transition of an explosive wave in the detonation. The derived formula is very simple, being also more suitable for studying the limiting processes of volume detonation. The conditions for the transition of a shock wave to a detonation wave are studied. Initial detonation conditions required for fast chemical reactions to take place at the front of a spherical explosive wave have been determined. A simple relation describing the critical detonation temperature for various pressures in the hydrogen-oxygen mixture was obtained. Using the known formulas for a shock transition, the critical temperature was coupled with the initial conditions in a static environment, such as the pressure, temperature, and hydrogen content in the mixture.

Keywords: detonation, point blast, spherical wave, Haber scheme, Lewis scheme, kinetics of chemical reactions, critical temperature

1. Introduction

The strong explosion in a small volume of a detonating gas mixture has been studied well in modern physics [1, 2]. The velocity of a detonation wave propagating in a spherical reactor can be calculated absolutely precisely with the use of a variety of original software programs [3]. There are also approximation formulas such as

$$\frac{D}{D_n} = 1 - \frac{A}{r - R_x}, \tag{1}$$

where r is the current radius, R_x is the critical radius, A is a constant, D_n is the velocity of a plane wave, and D is the velocity of a spherical wave. For larger charges, if the radius exceeds the critical one, the Eyring dependence

$$\frac{D}{D_n} = 1 - \frac{A}{r} \qquad (2)$$

is used. The work is aimed at analyzing the development of the process at the time moment, when the energy of a point explosion is equal to the energy of a burned gas, $r = R_x$, but provided that $R_x \neq \infty$. In other words, we intended to study the initial stage of detonation in reacting gas media by determining the scalar value of detonation wave velocity. The transition to the Chapman-Jouguet regime begins at some distance R_x from the center [4, 5], when the energy of the system appreciably increases. The model supposes that the pressures at the front and in the explosion region are equal, which results in the appearance of a high temperature at the transition point behind the shock front, since the main part of the substance mass is concentrated in a thin layer of the blast wave.

A lot of researches were devoted to the emergence of detonation in a hydrogen-oxygen mixture [6–8]. At the same time, there are no works in the scientific literature dealing with the influence of initial conditions on the detonation process, when the blast wave propagates in the gas environment. In this paper it was possible to obtain the necessary results by studying the chain reactions [9] of the interaction of hydrogen with oxygen.

2. Determination of the detonation wave velocity in an explosive gas mixture

2.1 Explosion in a chemically inert gas mixture

Consider an explosion in a chemically inert gas mixture. Let the point explosion occur instantly in a perfect gas with density ρ_0, and a shock wave propagates in the gas from the point of energy release. We intend to analyze the initial stage of the process of shock wave propagation, when the shock wave amplitude is still so high that the initial gas pressure, P_0, can be neglected. This assumption is equivalent to a neglect of the initial internal gas energy in comparison with the explosion one, i.e., we consider a strong explosion. The problem is to determine the velocity of the blast wave, when the wave front is modeled by a rigid piston compressing the volume of the gas in front (**Figure 1**). The main regularities of the process are well-known [10], and there is a simple approximate method to find them.

Let the total mass of a gas engaged into a blast wave be concentrated in a thin layer near the front surface. The gas density here is constant and equal to that at the front,

$$\rho_1 = \frac{\gamma + 1}{\gamma - 1} \rho_0. \qquad (3)$$

This formula can be derived from the formula for strong shock waves [11] in the case where the Mach number $M \gg 1$. To avoid a misunderstanding, note that, in this case, we mean a transformation of a medium denoted by subscript. 0 (the medium at rest before the explosion) into a medium denoted by subscript 1. The layer thickness Δr is determined from the condition of mass conservation,
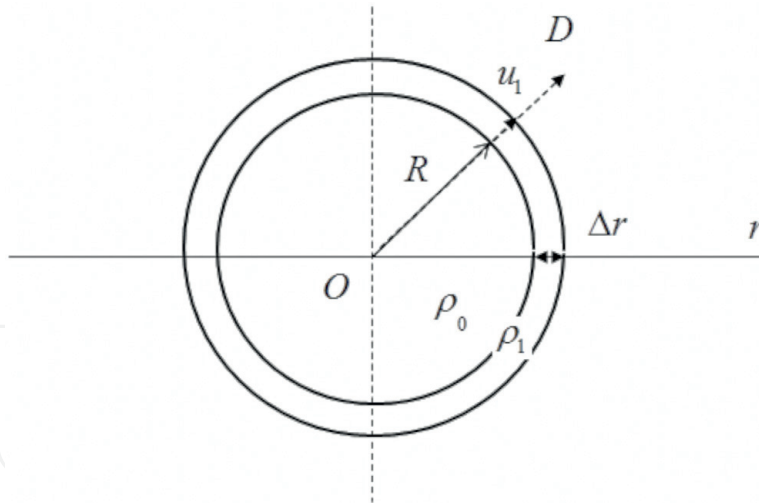
Figure 1.
Schematic diagram of a shock wave from the point explosion.

$$4\pi R^2 \Delta r \rho_1 = \frac{4}{3}\pi R^3 \rho_0; \tag{4}$$

whence

$$\Delta r = \frac{R\rho_0}{3\rho_1} = \frac{R}{3}\left(\frac{\gamma - 1}{\gamma + 1}\right). \tag{5}$$

Since the layer is very thin, the gas velocity in it almost does not change and coincides with that at the front,

$$u_1 = \frac{2D}{\gamma + 1}. \tag{6}$$

In the shock wave theory, a more accurate formula is considered, which couples the gas flow velocity behind the shock wave front, u_1, with the front velocity D: $u_1 = \frac{2D}{(\gamma+1)\left[1-\left(\frac{b_0}{D}\right)^2\right]}$, where b_0 is the sound velocity in the unperturbed gas. The gas mass in the layer is finite and equal to the mass m of the gas originally contained within a sphere of radius R,

$$m = \frac{4}{3}\pi R^3 \rho_0. \tag{7}$$

Let us denote the pressure at the inner layer side as P_c, and let it equal α times the pressure at the wave front, $P_c = \alpha P_1$. Newton's second law for the layer Δr in thickness reads

$$\frac{d}{dt}(mu_1) = 4\pi R^2 P_c = 4\pi R^2 \alpha P_1. \tag{8}$$

It can be used only within the limits

$$0 < R \leq R_x^0, \tag{9}$$

where the quantity R_x^0 is determined from energy considerations. At this point, the kinetic energy of the blast wave is still high enough, and its velocity considerably exceeds that of sound in the unperturbed gas medium.

3

Here, we arrive at a detailed mathematical representation of formulas and equations, by using the already known relations (4) and (8), which are the conservation laws for the mass and the moment, respectively. However, the latter are not enough for the problem to be solved. One more equation is needed,

$$E = E_T + E_k = const; \tag{10}$$

which is the energy conservation law. The explosion energy is constant and equal to a sum of two terms: the potential, E_T, and kinetic, E_k, energies. The general system consists of three equations—Eqs. (4), (8), and (10)—appended by the condition of strong explosion, $M \gg 1$, when formula (6), the relations (4), (8), (10) and the condition of strong explosion

$$M \gg 1 \tag{11}$$

are valid. Moreover, we have Eq. (6), and

$$P_1 = \frac{2}{\gamma + 1} \rho_0 D^2, \tag{12}$$

where P_1 is the pressure at the front of the shock wave. Formula (12) follows from the relation $\frac{P_1}{P_0} = \frac{2\gamma M^2 - \gamma + 1}{\gamma + 1}$ of work [11] in the case where $M \gg 1$: $\frac{P_1}{P_0} \approx \frac{2\gamma M^2}{\gamma + 1} = \frac{2\gamma \times \frac{D^2}{b_0^2}}{(\gamma + 1)} = \frac{2\gamma \times \frac{D^2 \rho_0}{\gamma P_0}}{(\gamma + 1)} = \frac{2\rho_0 D^2}{P_0 (\gamma + 1)}$.

It should be noted that, in the given system of equations, relation (4) does not determine a connection between the regions separated by the shock wave front (regions 0 and 1). Instead, it couples the states before the explosion and after it. While solving this problem for the one-dimensional centrally symmetric flow, we come back to Eq. (8).

The mass itself depends on the time, so that it is the momentum mu_1 rather than the velocity that should be differentiated with respect to the time. The mass is subjected to the action of the force $4\pi R^2 P_c$ directed from the inside, because the pressure P_c is applied to the inner side of the layer. The force acting from the outside is equal to zero, because the initial pressure of the gas is neglected. By expressing the quantities u_1 and P_1 in Eq. (8) in terms of the front velocity $D = \frac{dR}{dt}$ and using formulas (6) and (12), we obtain the new relation

$$\frac{1}{3}\frac{d}{dt}R^3 D = \alpha D^2 R^2. \tag{13}$$

Bearing in mind that

$$\frac{d}{dt} = \frac{d}{dR}\frac{dR}{dt} = D\frac{d}{dR} \tag{14}$$

and integrating Eq. (13), we find

$$D = aR^{-3(1-\alpha)} \tag{15}$$

where a is the integration constant. To determine the parameters a and α, let us take the energy conservation law into account. The kinetic energy of the gas is equal to

$$E_k = \frac{mu_1^2}{2}. \tag{16}$$

The internal energy is concentrated in a "cavity" confined by an infinitesimally thin layer. The pressure in the cavity is equal to P_c. Actually, this means that, strictly speaking, the whole mass is not contained in the layer. A small amount of the substance is included into the cavity as well. In gas dynamics, the specific internal energy of the ideal gas is calculated by the formula $e = \frac{P}{\rho}\left(\frac{1}{\gamma - 1}\right)$, where P is the pressure, ρ the density, and γ the adiabatic index. Therefore, the internal energy is equal to

$$E_T = \frac{1}{\gamma - 1} \times \frac{4\pi R^3}{3} P_c, \tag{17}$$

so that

$$E = E_T + E_k = \frac{1}{\gamma - 1} \times \frac{4\pi R^3}{3} P_c + \frac{mu_1^2}{2}. \tag{18}$$

Expressing the quantities P_c and u_1 once more in terms of D and substituting $D = aR^{-3(1-\alpha)}$, we obtain

$$E = \frac{4}{3}\pi\rho_0 a^2 \left[\frac{2\alpha}{\gamma^2 - 1} + \frac{2}{(\gamma + 1)^2}\right] R^{3 - 6(1-\alpha)}. \tag{19}$$

Since the explosion energy E is constant, the power exponent of the variable R must be equal to zero. This means

$$\alpha = \frac{1}{2}. \tag{20}$$

We determine the constant a from Eq. (19)

$$a = \left[\frac{3}{4\pi} \times \frac{(\gamma - 1)(\gamma + 1)^2}{3\gamma - 1}\right]^{\frac{1}{2}} \left(\frac{E}{\rho_0}\right)^{\frac{1}{2}}, \tag{21}$$

and substituting it together with Eq. (20) into formula (15), we arrive at the expression for the shock wave velocity in the case of point-like explosion

$$D = \left[\frac{3}{4\pi} \times \frac{(\gamma - 1)(\gamma + 1)^2}{3\gamma - 1}\right]^{\frac{1}{2}} \left(\frac{E}{\rho_0}\right)^{\frac{1}{2}} R^{-3/2}, \tag{22}$$

or

$$D = \xi_0 \left(\frac{E}{\rho_0}\right)^{\frac{1}{2}} R^{-3/2}, \tag{23}$$

where

$$\xi_0 = \left[\frac{3}{4\pi} \times \frac{(\gamma - 1)(\gamma + 1)^2}{3\gamma - 1}\right]^{\frac{1}{2}} = const. \tag{24}$$

2.2 Theory of explosion in a combustible mixture of gases

Distinctive features of the problem consist in that the exothermic chemical reactions are possible in such a medium. Therefore, it is quite reasonable to assume

that the blast wave continuously transforms into the detonation one. Let us consider the following model. An explosion in the gas generates a strong shock wave, which propagates over the gas and heats it up to a state, in which burning reactions become probable. We denote the energy of explosion by E_0. The energy U released at the combustion of the gas is equal t

$$U = \frac{4}{3}\pi R_1{}^3 \rho_0 Q', \quad R_0 \ll R_1 \tag{25}$$

where Q' is the specific heat released in the medium (per mass unit of the medium). The process is considered at the time moment t_1, when $R = R_1$ (**Figure 2**). Supposing that $E_0 > U$, we determine a condition, under which the detonation energy weakly affects the gas flow [12],

$$R_1 < R_x, \tag{26}$$

where $R_x^3 = \frac{3E_0}{4\pi Q' \rho_0}$. Let the charge have a finite radius R_0 Then, when applying the conventional theory of point explosion to the description of the motion, we have to use the estimation

$$R_0 < R < R_x. \tag{27}$$

It should be noticed that conditions (26) and (27) strongly restrict the scope, where the laws of point explosion in an inert gas are applicable to the flows in the detonating medium. However, if the energy $\boldsymbol{E_0}$ is high, and if it is released in a small volume, the flow in the region $\boldsymbol{R_1 < R_x}$ would mainly occur as it does at an ordinary point explosion. On the other hand, for the time moment $\boldsymbol{t_2}$, at which

$$R = R_2 \text{ and } E_0 < U, \tag{28}$$

the combustion processes start to play a dominating role, and the gas flow will possess the main characteristics of the detonation combustion [12].

From the aforesaid, some interesting conclusions can be drawn.

1. The theory of a point explosion is proposed to be used for a combustible mixture of gases within the limits $R_0 < R < R_x$, if the proposed model of transformation of a blast wave into a detonation one is valid for the given
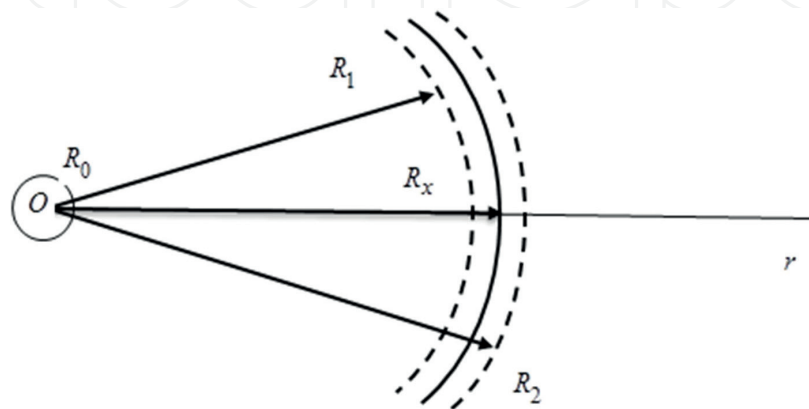

Figure 2.
Scenario of the continuous transformation of a blast wave into a detonation one: R_o is the charge radius, R_x is the initial threshold, R_2 is the final threshold, where the transformation of the strong detonation mode into the Chapman-Jouguet one is possible.

mixture. Another scenario is probable, when the detonation is impossible under the given physico-chemical conditions in the gas medium, and the blast wave simply fades.

2. When $R \to R_x$, the energy of the system considerably changes, $E \neq const$, increasing almost twice as much, which has to be taken into consideration while studying the gas motion at this stage.

3. It is evident that, if $R \to R_x$, the energy becomes proportional to the cube of the sphere radius, $E \sim R^3$.

Hence, we come to an idea of that, for the model of point explosion in a combustible mixture of gases to be valid at $R \to R_x$ under our conditions, it should be either modified or extended. Look once more at formula (19) expressing the energy conservation law. In the theory of point explosion for a usual non-detonable mixture of gases, it is adopted that $E = const$, which results in $\alpha = \frac{1}{2}$. However, in the case $\alpha = 1$, Eq. (19) yields $E \sim R^3$, which is necessary in our case. One can see that the energy conservation law allows the following set of relations:

$$\alpha = 1; \tag{29}$$

$$E = \frac{4}{3}\pi\rho_0 a^2 \left[\frac{2}{\gamma^2 - 1} + \frac{2}{(\gamma + 1)^2} \right] R^3; \tag{30}$$

$$a = \left[\frac{3(\gamma - 1)(\gamma + 1)^2}{16\pi\gamma} \right]^{\frac{1}{2}} \left(\frac{E}{\rho_0} \right)^{\frac{1}{2}} R^{-3/2}. \tag{31}$$

Substituting the new values of a and α into formula (15), we obtain

$$D = a = \left[\frac{3(\gamma - 1)(\gamma + 1)^2}{16\pi\gamma} \right]^{\frac{1}{2}} \left(\frac{E}{\rho_0} \right)^{\frac{1}{2}} R^{-3/2}. \tag{32}$$

According to the integration rules, the quantity a is a constant. Hence, a new formula for the velocity of a blast wave in the reacting gas medium is proposed:

$$D = \left[\frac{3(\gamma - 1)(\gamma + 1)^2}{16\pi\gamma} \right]^{\frac{1}{2}} \left(\frac{E}{\rho_0} \right)^{\frac{1}{2}} R^{-3/2} = const. \tag{33}$$

The law of conservation of energy gives unpredictable results, but these results are quite possible, given that the energy of the system is changing.

2.3 Formula for the velocity of a spherical wave

Let us determine the shock wave velocity in the critical zone, when $R \to R_x$ and $R \to R_2$ (**Figure 2**). One can consider a simplified version, when the transition occurs at a distance R_x from the center [4], but for the formation of normal detonation it is necessary to isolate the transition interval. As an example, let us consider the detonating gas, $2H_2 + O_2 = 2H_2O + Q$, where $Q = 286.5 \, kJ/mol$ is the thermal effect obtained at a combustion of one mole of hydrogen. Let this reaction (an initial explosion) be initiated. The energy of the system is

$$E = V n_{H_2} q + E_0, \tag{34}$$

where V is the volume of a certain ball, n_{H_2} the concentration of hydrogen molecules in it, q the thermal effect produced by one hydrogen molecule, and E_0 the initial energy of a charge of radius R_0 (recall that $R_0 \ll R_x$, but the current radius of the sphere $R \to R_x$). The volume of the ball and the concentration of hydrogen in it are calculated using the known formulas: $V = \frac{4}{3}\pi R^3$, $n_{H_2} = \frac{P_0}{K^* T_0} N_A c$, where $\frac{P_0}{K^* T_0} = \frac{\rho_0}{\mu}$; P_0, T_0, and ρ_0 are the initial pressure, temperature, and density of the gas mixture; K^* is the universal gas constant; N_A is the Avogadro constant; c the current content of hydrogen in the mixture (it is supposed that all the hydrogen burns out in the course of the reaction); and μ is the molar mass of the mixture. Hence,

$$E = \frac{4}{3}\pi R^3 \frac{P_0}{K^* T_0} N_A c q + E_0. \tag{35}$$

Substituting Eq. (35) into Eq. (33), we obtain

$$D = \left[\frac{(\gamma+1)^2(\gamma-1)N_A q c}{4\gamma\mu} + (\xi_0')^2 \frac{E_0}{\rho_0 R^3} \right]^{\frac{1}{2}},$$

where

$$\xi_0' = \left[\frac{3(\gamma-1)(\gamma+1)^2}{16\pi\gamma} \right]^{\frac{1}{2}}. \tag{36}$$

At the time moment, when $R \to R_2$, where $R_2 > R_x \gg R_0$, the second term in the brackets tends to zero, $(\xi_0')^2 \frac{E_0}{\rho_0 R^3} \to 0$, whence we obtain

$$D = \left[\frac{(\gamma+1)^2(\gamma-1)Q c}{4\gamma\mu} \right]^{\frac{1}{2}}, \tag{37}$$

taking into account that $Q = N_A q$, where Q is the thermal energy of one hydrogen mole. The final formula (37) is suggested to describe the velocity of a detonation wave. Above the threshold R_2, the charge energy E_0 loses its importance; further, the energy of the system is replenished only by the first term Eq. (35), which demonstrates the real wave velocity. Provided that formula (37) is valid, the examined quantity does not depend on the mixture pressure. At the initial time moment, the velocity is constant, and it is governed by the following parameters: the combustion energy per one mole of the combustible gas, Q; the fraction of the burned-out gas, c; the molar mass of the mixture, μ; and the adiabatic index for the given mixture of gases, γ.

For a plane wave, the following formula is widely known [11, 13]:

$$D = \sqrt{2(\gamma^2 - 1)Q^*} \tag{38}$$

where Q^* is the ratio between the energy released by a substance to the mass flow of this substance. As a result, by comparing formulas (37) and (38), we come to a conclusion that they are very similar, although the former seems to be more

Gas mixture	D_s [m/s]	D_n [m/s]	ε [%]
66.6%H_2+33.3%O_2	2550	2830	9.9
25%C_2H_2+75%O_2	2089	2330	10.3

Table 1.
Shock wave velocities.

adequate for the description of the spherical detonation at the beginning of the process. The results of calculations for two different gas mixtures are compared in the **Table 1**, where D_s is the velocity of a spherical wave calculated by the new formula (37) at the beginning of the detonation, when $R = R_2$; D_n is the plane wave velocity at the final stage of detonation, when $R \rightarrow \infty$, taken from work [14]; and ε is the corresponding relative difference.

In this work, the ideal case of the transformation of an explosive spherical wave into the Chapman-Jouguet mode is considered. From this viewpoint, formulas (33) and (37) prove that the regime of normal spherical detonation can exist at the beginning of the process, much earlier before the curvature radius can be assumed tending to the infinity. Moreover, it demonstrates a possibility of the existence of the normal spherical detonation with a lower velocity of a shock wave in comparison with the classical one. The mathematical expression (38) is "actual" at the final stage, when the radius tends to infinity, i.e. for the plane wave. It should be noted that, in the gas dynamics researches, instead of the shock wave velocity, its ratio to the sound velocity in the unperturbed gas medium, b_0, i.e. the Mach number M, is often used,

$$M = \frac{D}{b_0}. \tag{39}$$

With regard for the formula for the sound velocity,

$$b_0 = \sqrt{\gamma \frac{P_0}{\rho_0}} = \sqrt{\gamma \frac{K^* T_0}{\mu}}, \tag{40}$$

and expression (37), we obtain

$$M = \left[\frac{(\gamma + 1)^2 (\gamma - 1) Qc}{4\gamma^2 K^* T_0} \right]^{\frac{1}{2}}. \tag{41}$$

Formula (41) demonstrates the dependence of the Mach number on the adiabatic index γ, the combustion heat Q, the fraction of the burned-out gas c, and the temperature of the medium T_0. By varying those quantities, it is possible to regulate the shock transition intensity.
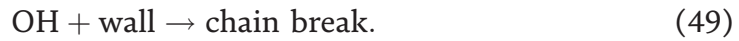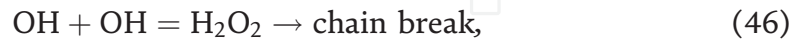
3. Conditions for the appearance of spherical detonation in the interaction of hydrogen with oxygen

3.1 Some issues concerning the chemical reaction kinetics

The process of shock wave propagation is very fast. For instance, at the shock wave velocity $D = 2500$ m/s and the gas layer thickness $r = 0.005$ m the shock compression of the substance lasts $t = 2 \times 10^{-6}$ s. This means that the dominant

part of a compressed substance must react within such a short time interval; only in this case, we may talk about the supersonic burning as a self-supporting process [13]. Proceeding from this viewpoint, let us consider some issues of the kinetics of the chemical reaction of H_2 and O_2.

First of all, it should be emphasized that the matter concerns chain reactions. The Haber scheme [9] and the development of a chain reaction with the Haber cycle look like

$$OH + H_2 = H_2O + H, \tag{42}$$

$$H + O_2 + H_2 = H_2O + OH, \tag{43}$$

$$H + O_2 = OH + O, \tag{44}$$

$$O + H_2 = OH + H, \tag{45}$$

$$OH + OH = H_2O_2 \rightarrow \text{chain break}, \tag{46}$$

$$H + H = H_2 \rightarrow \text{chain break}, \tag{47}$$

$$H + \text{wall} \rightarrow \text{chain break}, \tag{48}$$

$$OH + \text{wall} \rightarrow \text{chain break}. \tag{49}$$

Reactions (42) and (43) correspond to the chain continuation, reactions (44) and (45) to the chain branching, and reactions (46)–(49) to the chain break. For reaction (42), the corresponding activation energy is supposed to be high, with not every collision of OH and H_2 resulting in the reaction between them. On the contrary, reaction (43) runs at every ternary collision [9]. The cycle of reactions (42) and (43) composes a repeating chain link. According to Haber, 5–10, on the average, cycles must pass before reaction (44) occurs and there emerges a branching in the chain. Let us consider reactions (43) and (44), which compete with each other. Denoting the rate of reaction reaction (44) as W_3 and that of reaction (43) as W_2, the probability of branching δ can be defined as the rate ratio

$$\delta = \frac{W_3}{W_2}. \tag{50}$$

In Semenov's book [9], the expression for δ is given as

$$\delta = \frac{2.5 \times 10^5 \exp\left(\frac{-E_3}{K^* T_2}\right)}{[H_2]}, \tag{51}$$
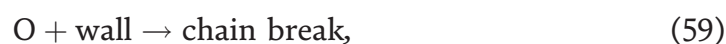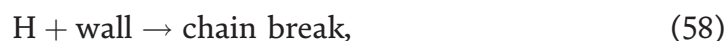
where $[H_2]$ is the partial pressure of hydrogen in units of mm Hg (the numerical coefficient of 2.5×10^5 in the nominator is multiplied by 1 mm Hg; therefore, the pressure in the denominator is expressed in terms of mm Hg units), E_3 is the activation energy of reaction (44), K^* the gas constant, and T_2 the medium temperature (in Kelvin degrees). According to Semenov's data [9, 15], $E_3 = 16$ kcal/mol. Formula (51) shows that δ strongly depends on the temperature, so that the process can be substantially accelerated as the temperature grows. Moreover, it turns out that the cycle of reactions (42) and (43) with branching (44) does not describe the fastest mechanism. There may exist a case where
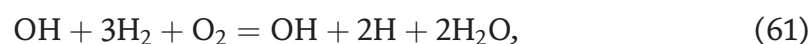
$$W_3 = W_2, \tag{52}$$

or

$$\delta = 1. \tag{53}$$

From the physical viewpoint, this means that the probability reaches the maximum, and the branching occurs at every chain link. Then the interaction scheme changes, reaction (44) substitutes reaction (43), and a transformation to the Lewis scheme takes place. In this case, we obtain $OH + H_2 = H_2O + H$, $H + O_2 = OH + O$, and so on, i.e. the temperature T_x, at which $\delta = 1$, is a critical one, when the kinetics of the interaction between hydrogen and oxygen undergoes qualitative changes. Let us write down the Lewis scheme in the complete form [9],

$$OH + H_2 = H_2O + H, \tag{54}$$

$$H + O_2 = OH + O, \tag{55}$$

$$OH + H_2 = H_2O + H, \tag{56}$$

$$O + H_2 = OH + H, \tag{57}$$

$$H + wall \rightarrow chain\ break, \tag{58}$$

$$O + wall \rightarrow chain\ break, \tag{59}$$

$$OH + wall \rightarrow chain\ break. \tag{60}$$

In the summarized form, the cycle reaction looks like

$$OH + 3H_2 + O_2 = OH + 2H + 2H_2O, \tag{61}$$

and just this reaction is associated with the first fastest initial chain transformations that give rise to detonation.

3.2 Medium state at the shock wave front. Critical temperature

Let a point explosion took place in a gas medium. In our case, the matter concerns the reacting gas media; therefore, the blast wave extinction may occur more slowly that usually; or it can be absent altogether, because a strong mechanism of chain reactions between hydrogen and oxygen starts to play its role. The ultimate result depends on the physico-chemical properties of the gas mixture and the initial energy of explosion. From this point of view, the most interesting is the model of a transition of the strong (overcompressed) detonation into the Chapman-Jouguet regime.

The shock wave propagates from a region with a higher pressure into a region where the pressure is lower. The gas dynamics usually considers waves that have a sharp front. The region of shock-induced transition is a discontinuous surface, the shock wave front. The unperturbed state is designated by subscript 1 and the perturbed one by subscript. 2. The density ρ, pressure P, and temperature T change in a jump-like manner across the front. The relations between the parameters (P_1, T_1, ρ_1) and (P_2, T_2, ρ_2) follow from the Hugoniot relations (the conservation laws) and the equation of ideal gas [11]. It is known that

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)M^2}{2 + (\gamma - 1)M^2}; \tag{62}$$

$$\frac{P_2}{P_1} = \frac{2\gamma M^2 - \gamma + 1}{\gamma + 1}; \tag{63}$$

$$\frac{T_2}{T_1} = \frac{(2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)}{(\gamma + 1)^2 M^2}, \tag{64}$$

where Mach number, M , $\gamma = \frac{C_p}{C_V}$ is the adiabatic exponent (for a two-atom ideal gas, γ =1.4 [16]). In such a manner, when a shock wave propagates in gases, we should consider the medium near (subscript 1) and at the front (subscript 2). To characterize the latter, we must know an important parameter, the shock wave velocity or the Mach number. In our case, using expression (37) and the formula for sound velocity (40), we obtain (41).

Now, let us carry out a simple gedanken experiment. Let a spherical reactor contain a hydrogen-oxygen mixture with the initial parameters (P_0, $T_0 = 293$ K). Let us heat up the mixture to the temperature $T_1 < T_1^*$, where T_1^* is the ignition temperature of the static medium. We initiate a reaction using an explosion and should observe a continuous transformation of a blast wave into the detonation of the hydrogen-oxygen mixture. At the wave front, the medium parameters are (P_2, T_2). Let

$$T_2 = T_x, \tag{65}$$

i.e. the critical temperature T_x is attained, and the reaction develops, being driven by the chain reaction mechanism according to the Lewis scheme. In order to determine the critical temperature T_x, let us use formula (51). Taking into account that $\delta = 1$, we obtain the transcendental equation for the critical temperature T_x

$$\frac{2.5 \times 10^5 \exp\left(-\frac{E_3}{K^* T_x}\right)}{[H_2]} = 1, \tag{66}$$

where

$$[H_2] = cP_2 \tag{67}$$

is the partial hydrogen pressure (in mm Hg units) at the shock wave front [17], P_2 is the total pressure in the mixture (in mm Hg units) at the shock wave front, and c the hydrogen content in the mixture (coefficient). With regard for Eq. (67), we obtain

$$\frac{2.5 \times 10^5 \exp\left(-\frac{E_3}{K^* T_x}\right)}{[cP_2]} = 1. \tag{68}$$

Let us express P_2 in the denominator of Eq. (68) in terms of known quantities. Before the reaction started (the initiation of the explosion), the gas mixture pressure was P_0, and its temperature was $T_0 = 293$ K. As the mixture is heated up to T_1, its pressure increases to

$$P_1 = P_0 \frac{T_1}{T_0}. \tag{69}$$

From Eq. (63), it follows that

$$P_2 = \frac{2\gamma M^2 - \gamma + 1}{\gamma + 1} P_1, \tag{70}$$

or, in view of Eq. (69),

$$P_2 = \frac{(2\gamma M^2 - \gamma + 1)P_0 T_1}{(\gamma + 1)T_0}. \tag{71}$$

The temperature T_1 in formula (71) is expressed in terms of T_x and the Mach number M as follows:

$$\frac{T_x}{T_1} = \frac{(2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)}{(\gamma + 1)^2 M^2}. \tag{72}$$

Whence, we obtain

$$T_1 = \frac{(\gamma + 1)^2 M^2 T_x}{(2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)}, \tag{73}$$

or, taking Eq. (73) into account,

$$P_2 = \frac{(\gamma + 1)M^2 T_x P_0}{T_0(2 + (\gamma - 1)M^2)}. \tag{74}$$

The denominator in formula (68) also includes the hydrogen content, c. If we assume that all hydrogen in the gas mixture burns out, we can express c using the Mach number (Eq. (41)) and the temperature of the gas medium T_1,

$$c = \frac{4\gamma^2 M^2 K^* T_1}{(\gamma - 1)(\gamma + 1)^2 Q}, \tag{75}$$

or, in accordance with Eq. (73),

$$c = \frac{4\gamma^2 M^4 K^* T_x}{(\gamma - 1)(2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)Q} \tag{76}$$

(in this case, we impose a restriction on the gas mixture composition, $0 < c \leq 0.66$). From Eq. (67) and using Eqs. (76) and (74), we obtain the partial pressure of hydrogen at the shock wave front,

$$[H_2] = \frac{4\gamma^2(\gamma + 1)M^6 K^* P_0}{(\gamma - 1)(2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)^2 Q T_0} T_x^2. \tag{77}$$

Then, formula (66) reads

$$T_x^2 = \frac{2.5 \times 10^5 Q T_0(\gamma - 1)(2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)^2}{4\gamma^2(\gamma + 1)M^6 K^* P_0} \exp\left(-\frac{E_3}{K^* T_x}\right). \tag{78}$$

Hence, we obtained the dependence which connects the initial pressure in the medium and the Mach number with the critical temperature at the shock wave front.

3.3 Results and discussion

After the substitution of the corresponding numerical values of physical parameters of the hydrogen-oxygen mixture and taking into account that $\gamma = 1.4$, $Q = 286.5 \text{ kJ/mol}$, $K^* = 8.31 \text{ J/(mol K)}$, $E_3 = 16 \times 10^3 \times 4.19 \text{ J/mol}$, and $T_0 = 293 \text{ K}$, Eq. (78) reads

$$T_x{}^2 = \frac{5.38 \times 10^{10} \left(2 + 0.4M^2\right)^2 \left(2.8M^2 - 0.4\right)}{P_0 M^6} \exp\left(-\frac{8067}{T_x}\right). \tag{79}$$

Most of these quantities are well known. The values of the others are chosen for practical reasons. So, for example, $T_0 = 293$ K, this is the temperature at which the experimental setup operates. The most optimal for laboratory conditions is the pressure of the gas mixture $P_0 = 60$ mm Hg, since at $P_0 > 60$ mm Hg the shock wave acquires destructive energy. Using expression (79), let us calculate the critical temperature for two Mach numbers, (i) $M = 2.15$ and (ii) $M = 4.78$, i.e. for shock waves of two types, but at the fixed initial pressure $P_0 = 60$ mm Hg. Experimental data indicate that detonation is not observed at $M < 2.15$, weak shock waves become waves of compression and rarefaction. At the same time, the value $M = 4.78$ was selected as the largest one obtained from expression (41) at the following parameters: $c = 0.66$, $T_1 = T_0 = 293$ K, and $\gamma = 1.4$. In the first case ($M = 2.15$ and $P_0 = 60$ mm Hg)

$$T_x{}^2 = 1.69 \times 10^9 \exp\left(-\frac{8067}{T_x}\right). \tag{80}$$

In the second one ($M = 4.78$ and $P_0 = 60$ mm Hg),

$$T_x{}^2 = 5.93 \times 10^8 \exp\left(-\frac{8067}{T_x}\right). \tag{81}$$

The transcendental equations were solved with the use of the software package "Consortium Scilab (Inria, Enpc)" with the program code "Scilab-4.1.2". After the corresponding calculations, we obtained $T_x = 1120$ K for the first case and $T_x = 1420$ K for the second one. The interval of researches can be expanded to determine the critical temperatures for Mach numbers within line segment [2; 5] with an increment of 0.2. Only real-valued roots, which have a physical sense, must be taken into consideration. The corresponding plot for the dependence $T_x \sim f(M)$ at $P_0 = 60$ mm Hg is shown in **Figure 3**.
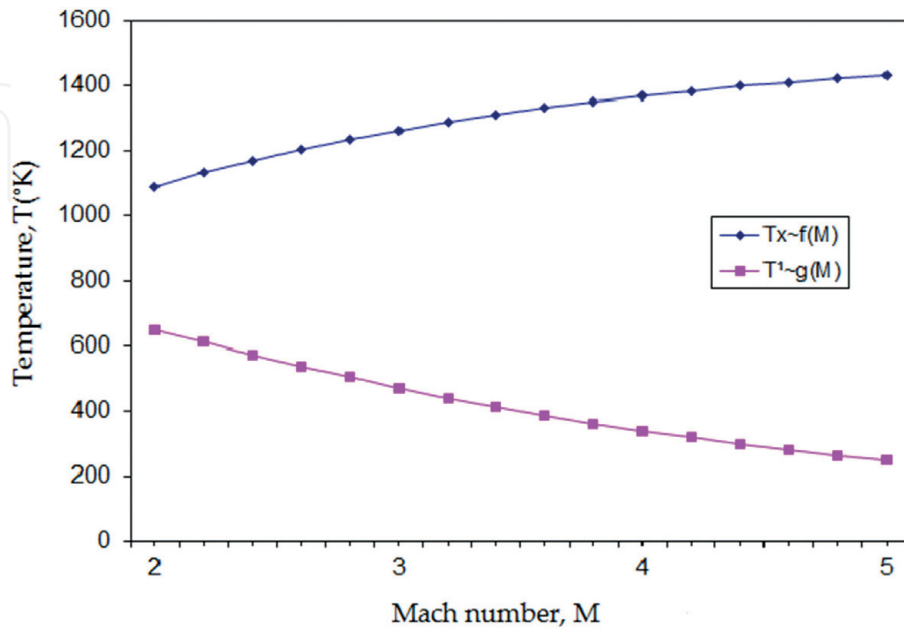

Figure 3.
Dependences of the critical temperature at the shock wave front, $T_x \sim f(M)$, and the temperature of static medium $T^1 \sim g(M)$, at which the detonation is possible, on the Mach number at a fixed pressure $P_0 = 60$ mm Hg.

One can see that the critical temperature grows nonlinearly with the Mach number. This behavior is not of surprise. The stronger the shock wave, the higher is the pressure at its front, and the higher is the probability of the chain break. As a result, we obtain the critical temperature growth, because the probability of chain break can be compensated only by the probability of chain branching, which increases with the medium temperature. However, this is not the main point. Knowing the critical temperature and the Mach number, it is possible to determine the initial temperature of the gas medium required for the detonation to take place. In other words, it is possible to determine such a temperature T^1 in front of the shock wave front that the corresponding wave would stimulate the detonation. Using expression (73), let us plot the dependence of T^1 on M at $P_0 = 60$ mm Hg (**Figure 3**). It allows us to determine the initial temperature of the medium, at which the detonation of the gas mixture becomes possible for the given Mach number. Moreover, in accordance with Eq. (41), the initial temperature and the known Mach number determine the hydrogen content. Hence, the critical temperature is unambiguously related with the Mach number and, therefore, with the initial parameters of the hydrogen-oxygen mixture.

4. Conclusions

To summarize, it should be noted that formula (37) determines the velocity of a detonation wave at the initial stage, if this wave is generated at the combustion of some "portion" (the parameter c) of a combustible gas, when $R \rightarrow R_2$ (see **Figure 2** and the model described the transformation of a blast wave in a detonation one). This formula is valid for spherical wave, in contrast to formula (38) known from the literature, which was obtained for plane waves. Thus, provided that the shock wave velocity or the Mach number is known, the solution of one of the basic gas dynamics problems can be obtained, i.e. we can find the parameters (P_1, T_1, ρ_1) at the wave front, if we know the set (P_0, T_0, ρ_0) of parameters for the unperturbed medium. In particular, the determined parameters are necessary for studying the kinetics of a chemical reaction in the course of the shock transition. There is no doubt that the stoichiometric mixture of hydrogen and oxygen will generate a detonation wave. However, it is difficult to assert the same for the mixture with 12% of hydrogen. In this case, it is necessary to consider the reaction mechanism itself.

The expression (66) obtained for the critical temperature is the simplest criterion for the transformation of the blast wave into a detonation one. At this temperature, $T_2 = T_x$ if $\delta = 1$, i.e. the probability of branching becomes maximum for the scheme of chain reactions with the hydrogen-oxygen interaction, which was considered above. The obtained Eq. (78) allows the sought value to be determined as a function of the Mach number, provided that the initial pressure is fixed. The critical temperature is the threshold of a detonation in a gas mixture, because the supersonic burning is impossible at temperatures below it. For example, let us analyze gas mixtures with different hydrogen contents of 66.6, 60, and 50%, and the temperature of static medium $T_1 = 273$ K (**Table 2**).

Gas mixture	T_1 [K]	M	T_2 [K]	T_x[K]
66.6%H$_2$ + 33.3%O$_2$	273	4.95	1558	1427
60%H$_2$ + 40%O$_2$	273	4.72	1438	1420
50%H$_2$ + 50%O$_2$	273	4.31	1241	1390

Table 2.
Parameter changes at the shock transition ($T_1 = 273$ K and $P_0 = 60$ mm Hg).

Gas mixture	T_1 [K]	M	T_2 [K]	T_x [K]
66.6%H_2 + 33.3%O_2	373	4.23	1648	1384
60%H_2 + 40%O_2	373	4.04	1523	1365
50%H_2 + 50%O_2	373	3.70	1339	1339

Table 3.
Parameter changes at the shock transition ($T_1 = 373$ K and $P_0 = 60$ mm Hg).

Comparing the T_2- and T_x-values, we come to a conclusion that the process, which is of interest for us, occurs only in the first two cases. However, it is enough to raise the initial temperature $T_1 = 373$ K for the detonation to become possible at lower hydrogen concentrations (**Table 3**).

The practical results testify that the conditions for the emergence of spherical detonation have a drastic dependence on the temperature and the mixture composition. The relation obtained in this work allows the critical values of those parameters to be determined and, in such a manner, to stimulate the regime of supersonic burning in the hydrogen-oxygen mixture. In the future, the presented results can be used to determine the range of admissible values of the parameters of the hydrogen-oxygen mixture necessary for detonation. Thus, it becomes possible to improve the performance of engines, make them more efficient.

Nomenclature

Basic designations

D	shock wave velocity, detonation velocity
R_x	critical radius
M	Mach number
P, T, ρ	pressure, temperature, density of the medium
u_1	gas velocity behind the shock front
b_0	speed of sound in a stationary gaseous medium
γ	adiabatic index
E_0	explosion energy
U	burnt gas energy
Q	combustion energy of one mole of combustible gas
μ	molar mass
K^*	universal gas constant
N_A	Avogadro number
c	coefficient of flammable gas content in the mixture
W	chemical reaction rate
δ	branching probability
$[H_2]$	is the partial pressure of hydrogen
T_x	critical temperature
H_2	hydrogen molecule
O_2	oxygen molecule
H_2O	water molecule
O	oxygen atom
H	hydrogen atom
OH	compound of an oxygen atom with a hydrogen atom
$f(x)$	function of the variable x
$\exp(x)$	exponential function

Δx	increment of variable x
$\frac{d}{dx}$	derivative
$\ll$	much less
$\gg$	much more
$\rightarrow$	aspires to
$[a; b]$	line segment

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