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Determination of Values Range of Physical Quantities and Existence Parameters of Normal Spherical Detonation by the Method of Numerical Simulation

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Abstract

Using elements of the theory of classical detonation and previously obtained relations for spherical waves, the author tried to establish the range of admissible values of temperature, Mach numbers, and specific hydrogen content in the gas mixture of the possible existence of normal spherical detonation. The work took into account the critical values of the parameters associated with the kinetics of the chemical reaction at the front of the blast wave and the parameters that determine the intensity of the shock transition (minimum and maximum Mach number) for a given reacting medium. Using the example of the interaction of hydrogen and oxygen in a hydrogen-oxygen mixture, it was possible to graphically determine the range of values of the main physical quantities and parameters - the critical temperature, the detonation temperature of the quiescent medium, and the specific hydrogen content in the mixture required for spherical detonation. Mathematical modeling of the process was carried out at a fixed value of the pressure of the gaseous medium.

Keywords: detonation wave, critical temperature, range of permissible values, process modeling

1. Introduction

Explosions are widely used in many areas of science and engineering, and their models are applied to elucidate various physical phenomena. Moreover, the unexpected explosions in industry and everyday life often result in catastrophes with numerous human losses, which invokes the intensive study of a supersonic burning nowadays. Those researches are carried out using both analytical methods [1] and numerical simulations [2, 3]. This work aims at studying the range of parameters needed for a normal spherical detonation in a gas mixture to take place. It is the kind of detonation that precedes the plane (classical) detonation, but emerges at lower shock wave velocities [4]. The spherical wave produced by a strong point explosion corresponds to the initial stage of the whole detonation process and transforms gradually into the classical variant. In gaseous explosive mixtures, the

detonation regime of the explosive transformation is possible only at certain concentrations of the combustible gas, depending on the chemical composition of the mixture, pressure and temperature. A decrease in pressure leads to the appearance of a pulsating detonation front, and subsequently to the formation of the so-called spin detonation, in which the three-shock wave configurations arising at the detonation wave front rotate along a helical line. With a further decrease in pressure, the supersonic combustion process dies out. At present, the reasons for the onset and existence of pulsating detonation [5] have not been fully investigated. It is hoped that in the near future this issue will be resolved after a detailed study of spherical detonation waves [6] and volumetric detonation.

In the earlier work [7], the model for the transition of an explosion spherical wave to the Chapman–Jouguet regime was proposed. In the other work [8], the concept of the critical temperature at the wave front was introduced as a basic criterion for the transformation of a shock wave to the detonation one. In this work, using the example of a gaseous hydrogen-oxygen mixture, an attempt is made to graphically determine the ranges of physical parameters and quantities at which spherical detonation is probable.

2. Critical values of parameters related to the chemical reaction kinetics

The classical theory considers detonation waves with sharp front edge. In its framework, the chemical transformations are assumed to begin right after a jump-like increase of the pressure. Actually, the process develops somewhat differently [9]. The temperature and pressure profiles behind the shock front of a detonation wave are schematically shown in **Figure 1**. After the shock transition (1–2), the vibrational and rotational degrees of freedom of gas molecules become excited (2–3), which is accompanied by a temperature reduction.

Then the induction period (3–4) takes place, the duration of which can be equal to more than 90% of the whole chemical reaction time (3–5), if the activation energy of the process is sufficiently high (E = 20 ÷ 40 kcal/mol). In the stationary detonation regime (the Chapman–Jouguet regime), profile 1–5 does not change in time. The reaction zone adjoins the region of non-stationary flow, rarefaction wave (5–6), the profile of which can change.
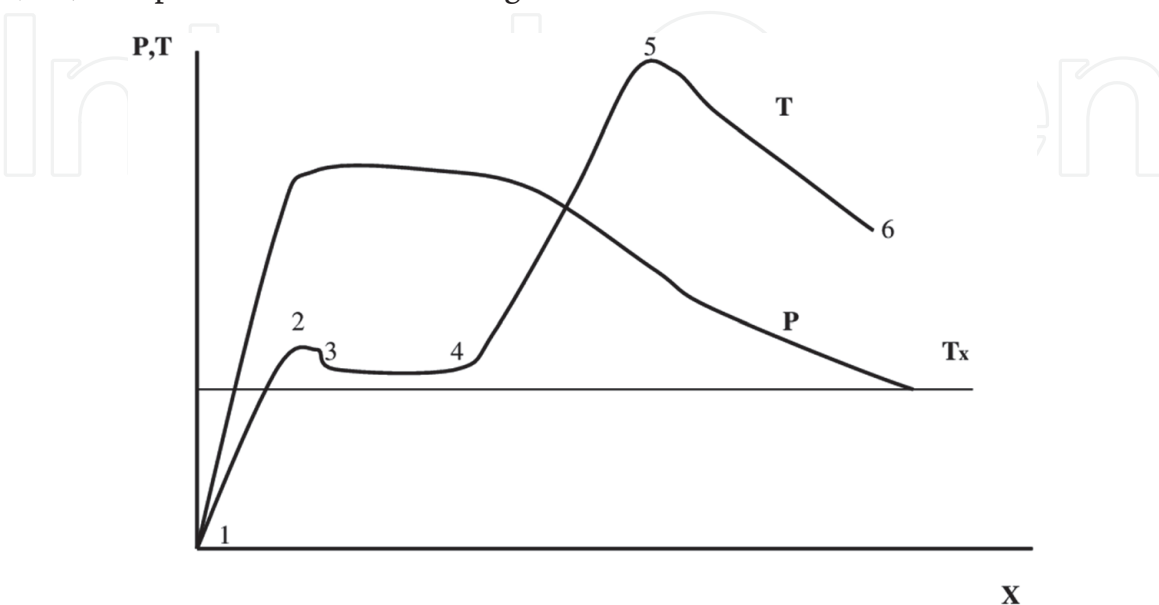

Figure 1.
Schematic diagrams of the pressure, P, and gas temperature, T, profiles behind the shock wave front [9] under the condition $T_2 \geq T_x$, where T_2 is the temperature at point 2.

It turns out that, in the case of a hydrogen-oxygen mixture compressed by a shock wave, a lot of free radicals emerge in section 2–4 [10, 11], with their concentration reaching $10^{12} \div 10^{15} \text{cm}^{-3}$. Rapid chain transformations start just from those initial centers [10] and run following the Lewis scheme. In this case, we have

$$OH + H_2 = H_2O + H, \tag{1}$$

$$H + O_2 = OH + O. \tag{2}$$
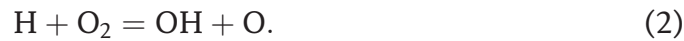
Note also that the temperature T_2, at which the branching probability δ equals unity,

$$\delta = 1, \tag{3}$$

is critical: the process becomes considerably accelerated, and the rapid chain reaction takes place. Under the indicated conditions, according to the results of work [4], the equality

$$T_2 = T_x, \tag{4}$$

plays the role of a criterion for qualitative variations in the kinetics of the interaction between hydrogen and oxygen. The Lewis scheme ignites the detonation mechanism, although the process itself can run in a certain different way, following a different scenario, in which the reaction rate is higher by an order of magnitude. From the chemical viewpoint, we have already stated the fact that, in order to obtain the supersonic burning at the shock wave front, it is necessary to reach the temperature T_x in the medium, at which the branching probability δ equals unity. How can T_x be determined? In work [4], the relation between the key parameters of a chemical reaction at the shock wave front, on the one hand, and the physical quantities that characterize the process of shock transition, on the other hand, was obtained,

$$T_x^2 = \frac{2.5 \times 10^5 Q T_0 (\gamma - 1)\left(2\gamma M^2 - \gamma + 1\right)\left(2 + (\gamma - 1)M^2\right)^2}{4\gamma^2(\gamma + 1)M^6 K^* P_0} \times exp\left(-\frac{E_2}{K^* T_x}\right), \tag{5}$$

where M is the Mach number (it reflects the shock transition intensity); P_0 the initial, before the explosion ignition (at 293 K), pressure of the gas mixture reckoned in mm Hg units; E_2 the activation energy of the branching reaction (2); K^* the gas constant; Q the combustion energy per gas mole; and γ the adiabatic index for the given gas mixture. For the hydrogen-oxygen mixture, the corresponding numerical values are [12]: $\gamma = 1.4$, $Q = 286.5$ kJ/mol, $K^* = 8.31$ J/mol/K, $E_2 = 16 \times 10^3 \times 4.19$ J/mol, and $T_0 = 293$ K. Then Eq. (5) reads

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

It is evident that the temperature T_x is different for different Mach numbers. Formula (6) describes the functional dependence of the critical temperature T_x on the Mach number M for the given initial pressure P_0 and allows one to compare its value with the real temperature

$$T_2 = \frac{\left(2\gamma M^2 - \gamma + 1\right)\left(2 + (\gamma - 1)M^2\right)}{(\gamma + 1)^2 M^2} \times T_1, \tag{7}$$

where T_1 is the temperature of the medium in front of the wave front. Hence, in our case, the important criterion,

$$T_2 \geq T_x, \tag{8}$$

has to be satisfied for the detonation to take place as a real process.

3. Elements of the hydrodynamic theory of detonation: limiting parameters dependent on the Mach number minimum and maximum

The detonation process of explosive materials is considered as a cumulative action of the shock wave and the chemical reaction, when the shock compression initiates the reaction, and the reaction energy maintains the detonation process afterward. The hydrodynamic theory [13] enables one to evaluate the size of a chemical reaction zone and the values of medium parameters in the chemical reaction zone (at the interface with the detonation products). The classical theory considers a plane detonation front,

$$d = \Delta t \left(D - v_g \right), \tag{9}$$

where d is the chemical reaction zone width, Δt the reaction duration, D the shock wave velocity, and v_g the gas velocity behind the reaction front (the Jouguet point). To be exact, in a real situation (**Figure 2**), there exists some shock transition interval (1–2) before the temperature T_2 is achieved, which is not taken into account in this case. One can see in **Figure 2** that front (3–3) separates the chemical reaction zone from detonation products. This means that the substance being suddenly compressed by the shock wave burns out completely within the time inter Δt.

The theory is based on two important postulates: (1) the whole substance compressed by the shock wave burns out, and (2) the combustion energy is enough to maintain the shock wave velocity to be constant ($D = const$). According to the theory, the pressure P_3 and the density ρ_3 in the chemical reaction zone at the interface with detonation products (the Jouguet point), are connected with each other by the following relations [13]:

$$P_3 = \frac{P_1 + \rho_1 D^2}{1 + \gamma}, \tag{10}$$

$$\frac{\rho_3}{\rho_1} = \frac{D^2(\gamma + 1)}{b_1^2 + \gamma D^2}, \tag{11}$$

Where P_3 is the pressure at front (3–3) separating the reaction zone from the reaction products, P_1 the pressure in front of the shock wave front, ρ_1 the gas density in front of the wave front, D the wave velocity, γ the adiabatic index, ρ_3 the medium density at the wave front (3–3), and b_1 the sound velocity in the motionless medium in front of the front. From the Mendeleev–Clapeyron equation

$$PV = \frac{m}{\mu} K^* T \Rightarrow T = \frac{P\mu}{\rho K^*}, \tag{12}$$

substituting the values of P_3 (10) and ρ_3 (11), we determine the temperature T_3 at the Jouguet point,
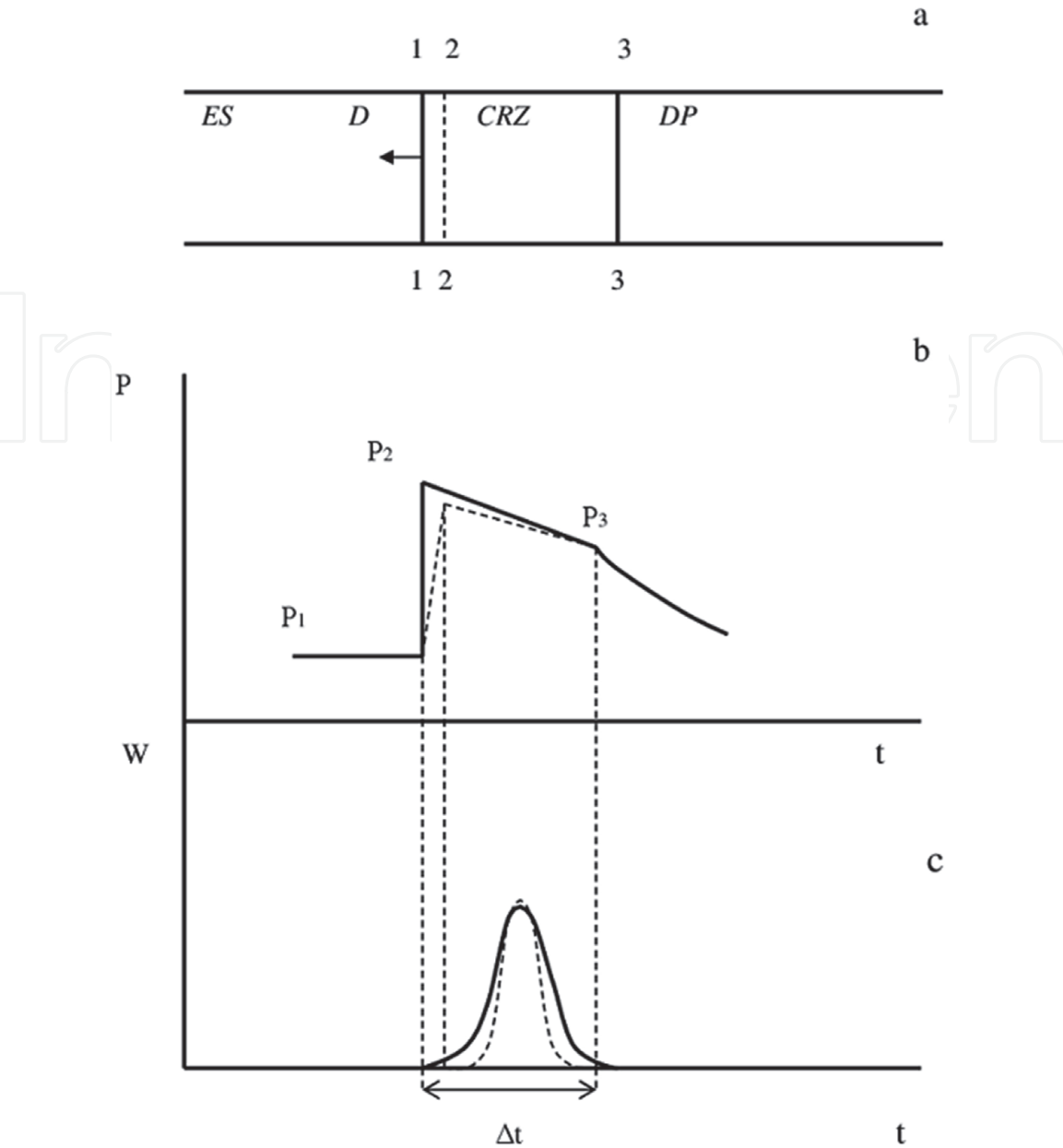
Figure 2.
Schematic structure of a plane detonation wave: explosive substance (ES), detonation products (DP), and chemical reaction zone (CRZ) (a). The pressure changing in time: in front of the wave front P_1, at the wave front P_2, and in the chemical reaction zone (the Jouguet point, P_3) (b). Reaction rates (c).

$$T_3 = \frac{\rho_1 D^2}{\gamma + 1} \times \frac{\mu}{K^*} \frac{\left(\gamma D^2 + b_1{}^2\right)}{\rho_1 D^2 (\gamma + 1)} = \frac{\mu\left(\gamma D^2 + b_1{}^2\right)}{K^* (\gamma + 1)^2} = \frac{\mu b_1{}^2}{K^*} \frac{\left(\gamma M^2 + 1\right)}{(\gamma + 1)^2} = T_1 \gamma \times \frac{\left(\gamma M^2 + 1\right)}{(\gamma + 1)^2},$$

$$(13)$$

where $D = b_1 M$. Here, we took into account that

$$P_3 \approx \frac{\rho_1 D^2}{\gamma + 1},$$

$$(14)$$

when $\frac{P_3}{P_1} \gg 1$, and that

$$b_1{}^2 = \gamma \frac{K^* T_1}{\mu},$$

$$(15)$$

where μ is the molar mass. It is evident that if we consider the detonation and the support of a chemical reaction by the shock wave, the following condition has to be satisfied:

$$T_3 > T_2; \qquad (16)$$

or, in a wider sense (**Figure 3**),

.
$$T_3 > T_2 > T_x \qquad (17)$$

Let us analyze inequality (16) in detail. From the theory of shock waves [13], it is known that the temperature at point 2 in **Figure 3** is determined by relation (7). Therefore, inequality (16) can be transformed as follows:

$$T_1 \gamma \frac{\gamma M^2 + 1}{(\gamma + 1)^2} > T_1 \frac{\left(2\gamma M^2 - \gamma + 1\right)\left(2 + (\gamma - 1)M^2\right)}{(\gamma + 1)^2 M^2} \qquad (18)$$

or

$$\gamma\left(\gamma M^2 + 1\right) - \frac{\left(2\gamma M^2 - \gamma + 1\right)\left(2 + (\gamma - 1)M^2\right)}{M^2} > 0, \qquad (19)$$

since $T_1 > 0$ and $\gamma > 0$. By solving the equation

$$\gamma\left(\gamma M^2 + 1\right) - \frac{\left(2\gamma M^2 - \gamma + 1\right)\left(2 + (\gamma - 1)M^2\right)}{M^2} = 0 \qquad (20)$$
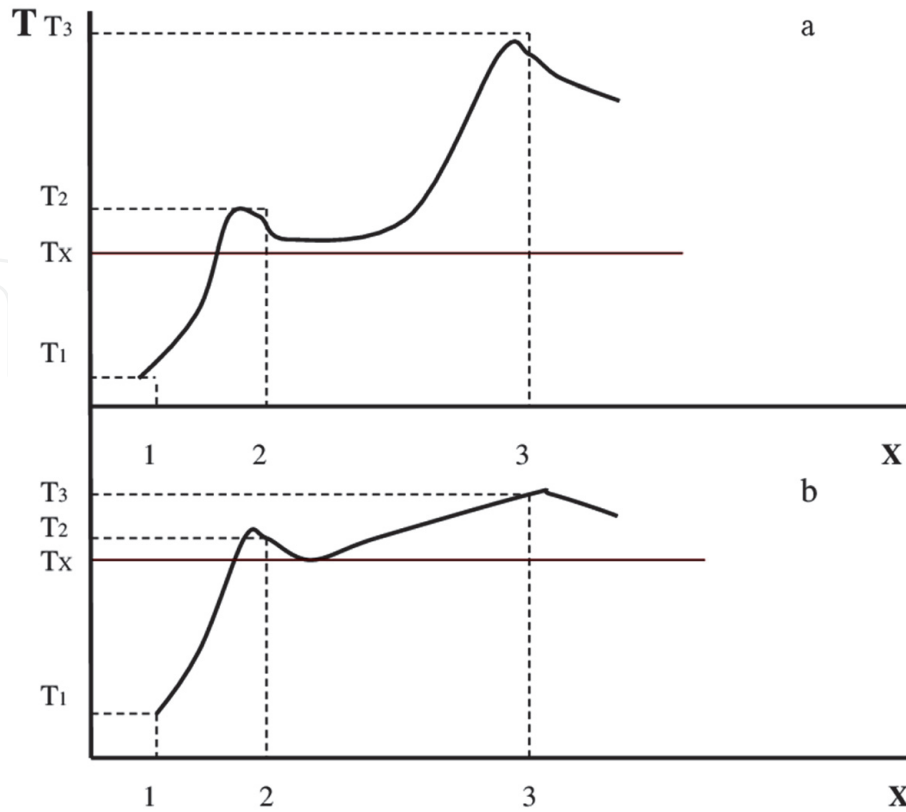

Figure 3.
Schematic diagrams for the temperature profiles behind the wave front: the general case (a) and the case where $T_3 \approx T_2 \approx T_x$ (b) corresponding to the limiting detonation process.

with respect to M (keeping in mind that $M > 0$), we obtain

$$M^4\left(2\gamma - \gamma^2\right) + M^2\left(\gamma^2 - 5\gamma + 1\right) + 2\gamma - 2 = 0 \qquad (21)$$

or, substituting the corresponding γ-value,

$$0.84M^4 - 4.04M^2 + 0.8 = 0. \qquad (22)$$

The positive roots of this equation are $M_1 = 2.145$ and $M_2 = 0.455$. For shock transitions, the most interesting is the first root, $M_1 = 2.145 \approx 2.2$. On the basis of inequality (18), we may assert that the detonation process is not possible for all shock waves, but only for those with the Mach number $M > 2.2$. Owing to hydrodynamic reasons, there is no detonation for waves with $M < 2.2$. While analyzing Eq. (20), it is expedient to admit that the temperature equality [14]

$$T_3 \approx T_2 \approx T_x \qquad (23)$$

describes the lower temperature limit of the detonation (**Figure 3**). In so doing, we took into account that the rate of the chemical reaction decreases together with the temperature in the chemical reaction zone. At the same time, according to the hydrodynamic theory, the amount of the substance that was compressed by the shock wave and interacted under its action has to remain at the previous level. This circumstance inevitably results in the time growth for the active reaction phase, and, as a consequence of the process continuity, gives rise to a considerable reduction of the induction period (interval 3–4 in **Figure 1**). In this connection, there emerges a possibility for the detonation wave to create a gas layer with an approximately identical temperature, and the Mach number $M \approx 2.2$ should be considered as the lower detonation limit.

In order to determine the upper limit of the detonation wave emergence by initiating an explosion in reacting gas media, let us use the model describing the continuous transition of a spherical explosion wave into the Chapman–Jouguet regime [4]. For the normal spherical detonation, it can be determined from the formula

$$M = \left[\frac{(\gamma + 1)^2(\gamma - 1)Qc}{4\gamma^2 K^* T_1}\right]^{\frac{1}{2}}, \qquad (24)$$

derived in work [4]. All quantities in this formula are known, except for the parameter c, the specific content of the burned out gas (hydrogen). The intensity of a detonation wave can be controlled by changing, mainly, two parameters: c (in the numerator) and T_1 (in the denominator). In our case, all hydrogen compressed by the shock wave burns out. The values of coefficient c are confined within the interval $0.66 \geq c > 0$. Let we have the stoichiometric mixture of hydrogen with oxygen ($c = 0.66 = max$), and the medium temperature $T_1 = -100\,^{\circ}C \approx 173K = min$. We suppose that a further temperature decrease will result in changes of the adiabatic index γ and the physical properties of the reacting mixture [15, 16], i.e. let formula (24) be valid for real gases at $T_1 \geq 173K$. In this case, we obtain a rough estimate for the Mach number maximum, $M_{max} = 6.2$. Note again that a strong explosion takes place in a cooled down medium. In this case, $M_{max} = 6.2$. Hence, we estimated the interval of possible Mach numbers for the normal spherical detonation of the hydrogen-oxygen gas mixture under real conditions:
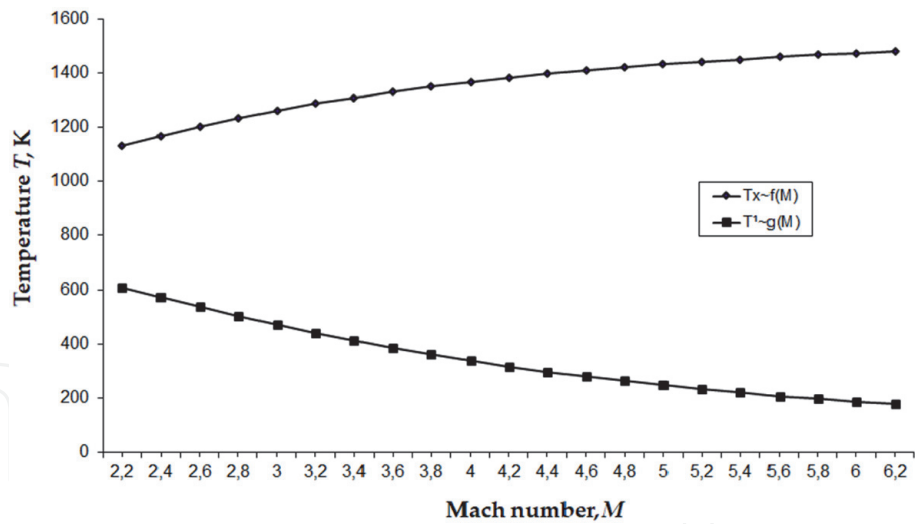
$$6.2 \geq M \geq 2.2. \qquad (25)$$

Figure 4.
Dependences of the critical temperature T_x and the detonation temperature in the motionless medium, T^1, on the Mach number M at the fixed pressure P = 60 mm Hg.

In view of relation (6), let us plot the dependence of the critical temperature on the Mach number, T_x (M) (**Figure 4**). Since the Mach number range was found, we will calculate the critical temperature T_x for every M from the indicated interval with an increment of 0.2 and the fixed initial pressure P_0 (see **Table 1**). Transcendental equations were solved using the "Consortium Scilab (Inria, Enpc)" software package with the "Scilab-4.1.2" code. When solving equations, only roots with real values that have physical meaning should be taken into account (the procedure was applied in [4]).

The larger the Mach number, the higher is the critical temperature. However, at $M \geq 5$, the critical temperature growth becomes a little slower. At the lower limit $M = 2.2$, $T_x = 1130\ K$, and, at the upper limit $M = 6.2$, $T_x = 1479\ K$. Hence, in a hydrogen-oxygen mixture, the critical temperature T_x for the allowable values of Mach number M accepts values from the following interval:

$$1479\ K \geq T_x \geq 1130\ K. \tag{26}$$

Figure 4 also exhibits the dependence of the detonation temperature T^1 on the Mach number M, which can easily be obtained [4] by substituting the critical temperature T_x into relation (7):

$$T^1 = \frac{(\gamma + 1)^2 M^2 T_x}{(2\gamma M^2 - \gamma + 1)\left(2 + (\gamma - 1)M^2\right)}. \tag{27}$$

From Eqs. (25) and (26), it follows that the detonation temperature for a motionless medium falls within the interval

M	2.2	2.4	2.6	2.8	3	3.2	3.4	3.6	3.8	4
T_x, [K]	1130	1166	1201	1233	1260	1286	1309	1329	1349	1365
T^1, [K]	609	572	537	503	470	440	412	385	360	337
4.2	4.4	4.6	4.8	5	5.2	5.4	5.6	5.8	6	6.2
1381	1396	1408	1420	1431	1441	1450	1458	1466	1473	1479
316	297	279	262	247	233	219	207	196	186	176

Table 1.
Values of critical temperature T_x and detonation temperature T^1 depending on the Mach number M ($P_0 = 60\ mm\ Hg$).

$$609 \, K \geq T^1 \geq 176 \, K. \tag{28}$$

This is the minimum temperature in front of the shock wave that makes the detonation possible.

4. Results of calculations and their discussion

Using the intervals obtained above for some physical quantities, let us graphically determine the region of existence for the normal spherical detonation. The upper limit of the hydrogen content in the mixture is confined in our case by the value $c = 0.66$. Above this value, the chemical reactions resulting from the interaction between hydrogen and oxygen in the mixture, which were considered in work [4], become more complicated, and this circumstance may result in different values of critical temperature. Further researches of this issue are required. Below, the choice $T_1 = 800 \, K$ for the upper limit of the medium temperature is explained in detail.

With regard for dependence (24) of the Mach number M on the temperature of a motionless medium T_1 and the hydrogen content c, let us plot the dependences $M(c)$, $T_x(c)$, and $T^1(c)$ at fixed T_1 and P_0. We proceed from the plots of the dependence $M(c)$ at $T_1 = const$ exhibited in **Figure 5** for T_1-temperatures in the interval $800 \, K \geq T_1 \geq 173 \, K$ (see **Table 2**). The lower curve corresponds to the gas mixture temperature $T_1 = 800 \, K$, and the upper one to $T_1 = 173 \, K$. According to expression (24), this family of curves has a power dependence on the hydrogen content in the mixture, c, with a power exponent of 0.5. Let us fix the maximum content of burned out hydrogen, $c = 0.66$, which corresponds to the stoichiometric composition of hydrogen-oxygen mixture, and draw a vertical line. The Mach number corresponding to its intersection with the mentioned family of curves changes from $M = 2.8$ at point 4 to $M = 6.2$ at point 5. Another important detail should be emphasized. Four dashed lines are drawn in **Figure 5**. Two horizontal
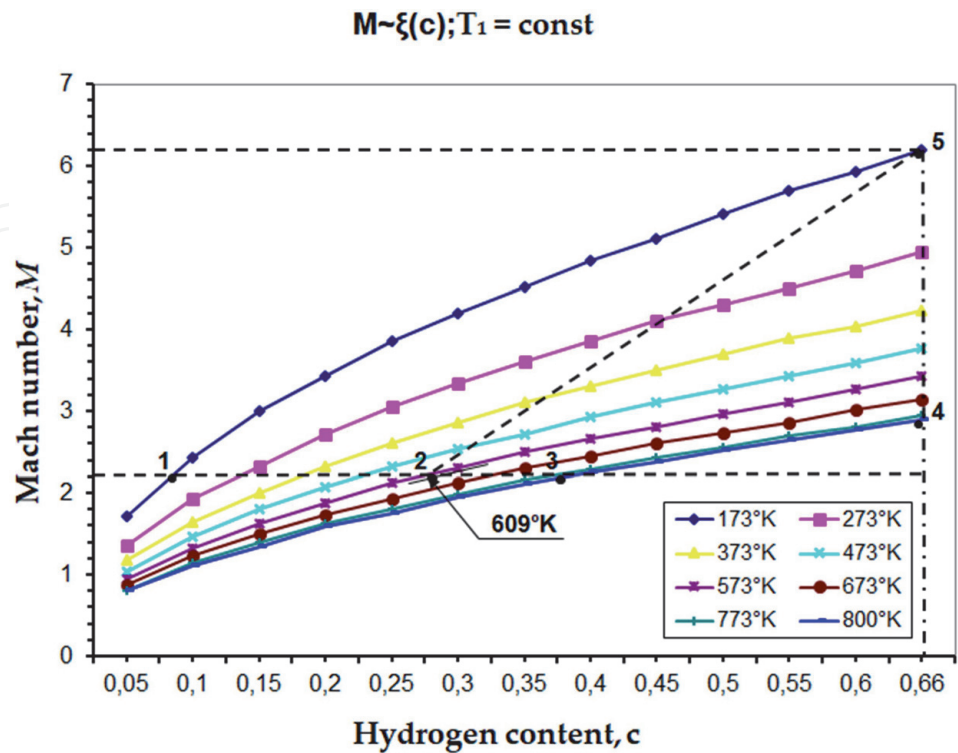

Figure 5.
Dependence of the Mach number M on the hydrogen content c in the gas mixture ($P_0 = 60 \, mm \, Hg$) for various temperatures in the motionless medium, T_1.

	c	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.66
173°K	M	1.71	2.42	3	3.42	3.85	4.19	4.51	4.84	5.1	5.41	5.7	5.93	6.2
273°K		1.36	1.93	2.32	2.72	3.05	3.34	3.6	3.85	4.1	4.31	4.5	4.72	4.95
373°K		1.17	1.65	2	2.33	2.6	2.85	3.1	3.3	3.5	3.69	3.9	4.04	4.23
473°K		1.03	1.46	1.8	2.07	2.32	2.53	2.72	2.93	3.1	3.27	3.42	3.59	3.76
573°K		0.94	1.33	1.62	1.88	2.12	2.3	2.5	2.66	2.81	2.97	3.1	3.26	3.42
673°K		0.87	1.23	1.5	1.74	1.93	2.13	2.3	2.45	2.6	2.74	2.86	3.01	3.15
773°K		0.81	1.14	1.39	1.62	1.8	1.98	2.16	2.29	2.43	2.56	2.7	2.81	2.94
800°K		0.8	1.11	1.34	1.59	1.75	1.95	2.11	2.25	2.38	2.52	2.64	2.76	2.89

Table 2.
Data of the Mach number M, depending on the specific content of hydrogen c at $T_1 = const$, $P_o = 60\ mm\ Hg$.

ones confine the region of allowable Mach numbers corresponding to the normal spherical detonation. The first line corresponds to the minimum $M_{min} = 2.2$, and the second one to the maximum $M_{max} = 6.2$. The third dashed vertical line corresponds to the stoichiometric composition of the hydrogen-oxygen mixture and is the optimal variant for the detonation. The fourth line will be discussed below.

Let us consider points 1 to 5 in **Figure 5** separately. Segment 1–2 corresponds to the lower limit of the shock wave velocity $M_{min} = 2.2$, but the medium temperature for the segment points turns out lower than the detonation one (**Figure 4**). Therefore, the detonation is impossible in this case. The region of the probable detonation for this Mach number is restricted to segment 2–3, because the temperature of motionless medium reaches the detonation temperature values here. On the basis of **Figure 4**, it is also possible to draw a conclusion that, for the medium temperature $T_1 = 173\ K$, the detonation is possible if $M = M_{max} = 6.2$ (point 5 in **Figure 5**). In other words, for the chosen temperature, $800\ K \geq T_1 \geq 173\ K$, and hydrogen content, $0.66 \geq c \geq 0.075$, intervals, the region of the probable detonation is bounded by segments 2–3, 3–4, 4–5, and 5–2. Segment 5–2 is presented in **Figure 5** schematically by a straight line. In the general case, in view of the nonlinear dependence $M(c, T_1)$, this segment is curvilinear.

Let us derive the functional dependence $T_x(c)$ by substituting the $M(c)$ dependence (Eq. (24)) into Eq. (5). To make transformations simpler, let us rewrite Eq. (24) in a slightly different form,

$$M = [\eta c]^{\frac{1}{2}}, \tag{29}$$

where

$$\eta = \frac{(\gamma + 1)^2 (\gamma - 1) Q}{4\gamma^2 K^* T_1}. \tag{30}$$

Then we obtain the following transcendental equation for the critical temperature T_x:

$$T_x^2 = \frac{2.5 \times 10^5 Q T_0 (\gamma - 1)(2\gamma\eta c - \gamma + 1)(2 + (\gamma - 1)\eta c)^2}{4\gamma^2 (\gamma + 1) K^* P_0 \eta^3 c^3} \times \exp\left(-\frac{E_2}{K^* T_x}\right) \tag{31}$$

or, taking Eq. (30) into account,

$$T_x^2 = \frac{2.5 \times 10^5 T_0 T_1 (2\gamma\eta c - \gamma + 1)(2 + (\gamma - 1)\eta c)^2}{(\gamma + 1)^3 P_0 \eta^2 c^3} \exp\left(-\frac{E_2}{K^* T_x}\right). \tag{32}$$

In **Figure 6**, using expression (32) and **Table 3**, we plotted the dependences $T_x(c)$ at $P_0 = const$ and $T_1 = const$. By the form, they are similar to the previous plots (**Figure 5**) and confirm the conclusions made for points 1 to 5.

More interesting is the dependence of the detonation temperature in the motionless medium on the hydrogen content, $T^1(c)$, at $P_0 = const$ and $T_1 = const$. It can be determined from relation (5) with regard for Eqs. (7) and (4):

$$
(T^1)^2 = \frac{2.5 \times 10^5 Q T_0 (\gamma - 1)(\gamma + 1)^3}{4\gamma^2 K^* P_0 (2\gamma M^2 - \gamma + 1) M^2}
$$
$$
\times \exp\left(-\frac{E_2(\gamma + 1)^2 M^2}{K^* T^1 (2\gamma M^2 - \gamma + 1)(2 + (\gamma - 1)M^2)}\right). \tag{33}
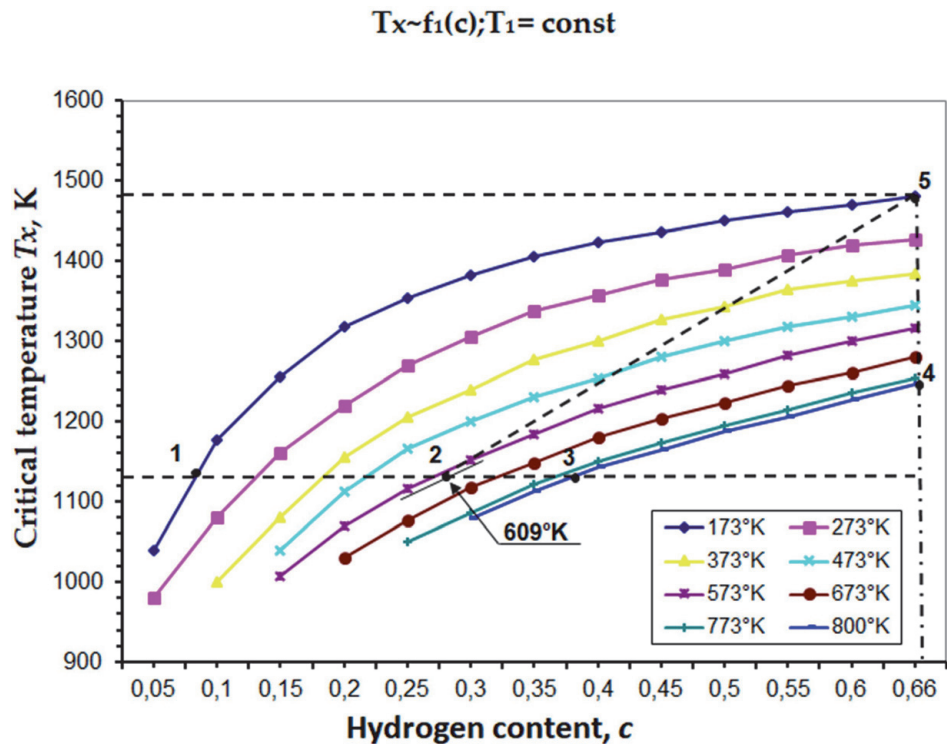$$

Figure 6.
Dependences of the critical temperature T_x on the hydrogen content c in the gas mixture ($P = 60$ mm Hg) for various temperatures in the motionless medium, T_1.

c		0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.66
173°K	T_x	1040	1176	1256	1317	1354	1382	1405	1423	1436	1450	1460	1470	1480
273°K		980	1080	1160	1220	1270	1305	1338	1358	1376	1390	1408	1420	1427
373°K			1000	1080	1155	1205	1240	1276	1300	1327	1343	1364	1375	1384
473°K				1040	1113	1166	1200	1230	1254	1280	1300	1318	1330	1344
573°K				1008	1070	1116	1152	1184	1216	1240	1259	1282	1300	1316
673°K					1030	1076	1118	1148	1180	1204	1223	1244	1260	1280
773°K						1050	1085	1122	1150	1174	1195	1215	1236	1253
800°K							1078	1112	1142	1164	1187	1205	1226	1246

Table 3.
Data showing the functional dependence of the critical temperature T_x on the specific content of hydrogen c at $T_1 = const$, $P_0 = 60$ mm Hg.

Making allowance for Eqs. (29) and (30), relation (33) can be simplified to the following form:

$$\left(T^1\right)^2 = \frac{2.5 \times 10^5 T_0 T_1 (\gamma + 1)}{cP_0(2\gamma\eta c - \gamma + 1)} \times \exp\left(-\frac{E_2(\gamma + 1)^2 \eta c}{K^* T^1 (2\gamma\eta c - \gamma + 1)(2 + (\gamma - 1)\eta c)}\right).$$

(34)

The corresponding family of curves is shown in **Figure 7**, according to **Table 4**. While analyzing the plots, the attention should be drawn to the following facts. (i) Every temperature T_1 of the gas mixture is associated with a specific dependence
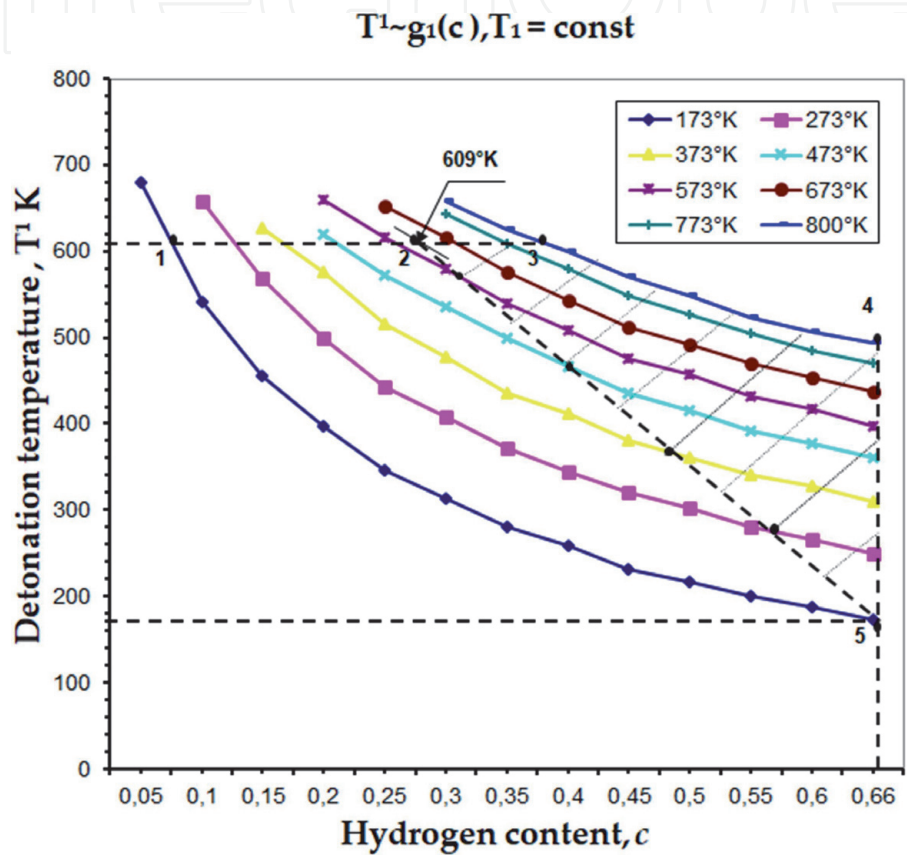

Figure 7.
Diagrams of the dependence of the detonation temperature T^1 on the hydrogen content c in an explosive gas mixture $H_2 + O_2$ (P = 60 mm Hg) for different temperatures in a stationary environment, T_1.

	c	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.66
173°K	T^1	680	542	456	398	346	313	280	258	232	217	200	188	173
273°K			658	568	500	442	409	372	345	320	302	280	266	250
373°K				626	576	516	477	436	412	381	360	340	328	310
473°K					620	572	535	500	467	436	416	392	378	360
573°K						660	616	580	540	508	476	458	432	418	398
673°K							652	616	576	543	512	492	470	454	438
773°K								644	609	580	548	526	504	484	470
800°K								658	625	600	570	548	523	507	493

Table 4.
Values of the detonation temperature T^1, depending on the specific content of hydrogen c at T_1 = const, P_o = 60 mm Hg.

$T^1(c)$. (ii) As the hydrogen content in the mixture grows, the temperature of the detonation T^1 in the motionless medium drastically decreases, which is especially appreciable at low temperatures. (iii) Let us draw a horizontal line that intersects the family of curves (for example, let it be the dashed line $T^1 = 173\ K$). At the point of its intersection with the curve corresponding to the same temperature of the motionless medium (in our case, this is $T_1 = 173\ K$), the detonation condition $T_2 = T_x$ (point 5) is satisfied. Detonation becomes probable, because the current temperature of motionless medium reaches the detonation temperature for this medium ($T_1 = T^1$). (iv) The intersection points of any horizontal line (see item iii) correspond to the critical hydrogen contents in the mixture, below which the detonation is impossible. The dashed line connecting points 2 and 5 in **Figure** 7 corresponds to the condition $T_2 \geq T_x$ for the whole family of curves.

Let the hydrogen content in the mixture change from 0.075 (point 1) to 0.66 (point 4). Then, on the basis of the plots shown in **Figure** 7, one may assert the following.

1. As was indicated above, a temperature lower than $T^1 \approx 173 \div 176\ K$ can give rise to a variation in the physical properties of the reacting mixture. Then the proposed formulas will produce erroneous results. The horizontal dashed line that passes through point 5 corresponds to this temperature, and point 5 testifies to the explosion with the maximum Mach number $M_{max} = 6.2$.

2. According to the plot of the functional dependence $T^1(c)$ at $T_1 = 273\ K$ (see Eq. (34) and **Figure** 7), the detonation is possible if the hydrogen content in the mixture is not lower than 0.57.

3. Physical restrictions imposed by the minimum Mach number $M_{min} = 2.2$ bring about the existence of the upper limit for the detonation temperature, $T^1 = 609\ K$. Points of both segments 1–2 and 2–3 correspond to the allowable values of Mach number. However, the detonation is possible only for the points on segment 2–3, because the main condition $T_2 \geq T_x$ is satisfied at $T_1 \geq 609\ K$. Whence it follows that $c = 0.27$ is the minimum hydrogen content in the mixture, below which the detonation is mpossible even at very high temperatures.

4. Experimental results testify that, if the temperature of a gas mixture is higher than $T_1 = 800\ K$, the spontaneous ignition takes place, which can transform into the detonation, if the hydrogen content in the mixture is not lower than 0.37. Therefore, this temperature is a kind of upper limit, to which the hydrogen-oxygen mixture can be heated.

From the reasons given above, it follows that the region of spherical supersonic burning is bounded by segments 2–3, 3–4, 4–5, and 5–2 in **Figure** 7. For the illustrative purpose, it was hatched.

5. Conclusions

The dependences between the temperature, Mach number, the hydrogen content in the hydrogen-oxygen mixture as the main parameters characterizing the process of transformation of a shock wave into a detonation one and affecting the chemical reactions between reacting components are studied. On the basis of

relations obtained earlier [4], the conditions are found, under which the probability of a chain branching reaches unity ($\delta = 1$), and a fast chain reaction is started. The existence of the critical temperature T_x at the front of a shock wave, above which the detonation takes place, is substantiated, as well as the functional dependence (5) of the critical temperature on the Mach number. In author's opinion, the latter should be taken as a basis, while studying the processes of spherical detonation. Summarizing the results of work [4], the ondition $T_2 \geq T_x$ is found, which connects the kinetics of a chemical reaction with the detonation in a gas mixture. On the basis of the relations of the hydrodynamic theory of detonation, the region of possible values for the temperatures at the shock wave front, T_2, and in the chemical reaction zone, T_3, is determined. The equality $T_x \approx T_2 \approx T_3$ which couples them, corresponds to the lower limit, at which the detonation is possible. The minimum and maximum values of Mach number in reacting gas media are also determined, which enables the process of supersonic burning to be analyzed in more details and the region of physical parameters and quantities (the critical emperature, the temperature of detonation in the motionless medium, and the hydrogen content in the mixture), at which the spherical detonation is probable, to be indicated. The latter is llustrated, by using the hydrogen-oxygen mixture as an example.

To summarize, it should be noted that this paper is final in a cycle of works devoted to the study of the whole process of normal spherical detonation.

Acknowledgements

Nomenclature

Basic designations:

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
T_x	critical temperature
T_2	temperature at the shock front
δ	branching probability
D	shock wave velocity, detonation velocity
M	Mach number
P, T, ρ	pressure, temperature, density of the medium
ES	explosive substance
DP	detonation products
CRZ	chemical reaction zone
γ	adiabatic index
Q	*combustion energy of one mole of combustible gas*
μ	*molar mass*
K^*	*universal gas constant*
E_2	the activation energy of the branching reaction

d	the chemical reaction zone width
Δt	the reaction duration
v_g	the gas velocity behind the reaction front
b_1	the sound velocity in the motionless medium in front of the front
m	gas mass
T_3	temperature at the Jouguet point
c	coefficient of flammable gas content in the mixture
W	chemical reaction rate
T^1	detonation temperature
M_{max}	maximum Mach number
M_{min}	minimum Mach number
$f(x)$	function of the variable x
$\exp(x)$	exponential function
Δx	increment of variable x
$\ll$	much less
$\gg$	much more
$\approx$	almost equal
$[a;b]$	line segment

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References

[1] Orlenko L. P, editor. Physics of Explosion. 3rd ed. Moscow: Fizmatlit; 2004. V.1. 832 p.

[2] Mader, C. Numerical Simulation of Detonation. 1st ed. Berkeley: University of California; 1979. 485 p.

[3] Fedorov A. V, Tropin D. A, and Bedarev I. A. Mathematical modeling of the suppression of the detonation of a hydrogen-oxygen mixture by inert particles. Fiz. Goren. Vzryva. 2010; 46 (3):103–115.

[4] Myron Polatayko (November 5th 2018). Determination of the Velocity of the Detonation Wave and the Conditions for the Appearance of Spherical Detonation during the Interaction of Hydrogen with Oxygen [Online First], IntechOpen, DOI: 10.5772/intechopen.81792. Available from: https://www.intechopen.com/online- first/determination-of-the-velocity-of-the-detonation-wave-and-the-conditions-for-the- appearance-of-spheri

[5] Kasimov A.R., Faria L.M., Rosales R. R. On a Theoretical Prediction of the Dynamics of Pulsating and Cellular Detonations in Gases. Combustion and Explosion. 2016; 9 (2): 42–50

[6] Myron Polatayko. Features of Spherical Detonation in Explosive Gas Environments, Public Science Framework, Physics Journal. 2019; 5(1): 1–7. Available from: http://www.aiscience.org/journal/allissues/pj

[7] Polatayko M. M. Determination of detonation wave velocity in an explosive gas mixture. Ukr. Fiz. Zh. 2012; 57(6): 606–611.

[8] Polatayko, M.M. Conditions for the Occurrence of Spherical Detonation in a Hydrogen- Oxygen Mixture. Ukr. Fiz. Zh.. 2013; 58 (10): 963–968.

[9] Soloukhin R. I. Shock Waves and Detonations in Gases. Baltimore: Mono Books; 1966. 176p.

[10] Semenov N. N. Chemical Kinetics and Chain Reactions. Oxford: Clarendon Press; 1935. 480 p.

[11] Semenov N. N. Some Problems of Chemical Kinetics and Reactivity. Princeton: Princeton Univ. Press; 1959. V.1. 254 p.

[12] Matveev A. N. Molecular Physics. Moscow: Mir Publishers; 1985. 450 p.

[13] Sysoev N. N, and Shugaev F. V. Shock Waves in Gases and Condensed Media. Moscow: Moscow State University; 1987. 133 p.

[14] Polatayko M. M. Possibility of Normal Spherical Detonation in a Hydrogen-Oxygen Gas Mixture: Allowable Temperature, Mach Number, and Hydrogen Content. Ukr. Fiz. Zh. 2014; 59(10):980–988.

[15] Ravdel A. A, Ponomareva A. M, editors. A Brief Handbook of Physico-Chemical Values. Eighth ed. Leningrad: Khimiya; 1983. 232 p.

[16] Morachevsky A. G., Sladkov I. B. Physico-Chemical Properties of Molecular Inorganic Compounds. Leningrad: Khimiya; 1987. 192p.