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Features of Spherical Detonation in Explosive Gas Environments

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Abstract

In one of the previous works, using the theory of explosion and the laws of conservation of mass, momentum and energy, the author managed to solve the system of equations for the spherical detonation model. The possible existence of a stationary mode at the beginning of the transition of a blast wave to detonation was proved, and a new formula appeared that determines the speed of a spherical detonation wave in reacting gases. This served as a powerful incentive for further studies of the detonation process. The proposed article is a logical continuation of the previous works. The main attention in the article is drawn to the fact of instability of the normal spherical detonation and instability of the Chapman-Jouguet regime, when the radius of the wave front considerably exceeds the critical one. The author studies the reasons for the increase in the speed of a spherical detonation wave during its transition to plane wave at large distances from the center of the explosion. The possibility of transition of a normal spherical detonation to a more stable state, with a higher energy level, in the form of a flat stationary detonation is indicated. It is assumed that two stationary states exist, that is, two energy levels for the stationary detonation, which makes it possible to explain the phenomenon of pulsating detonation in gaseous media.

Keywords

Normal Spherical Detonation, Unstable State, Eyring Formula, Wave Speed, Steady State, Energy Levels, Pulsating Detonation

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1. Introduction

Spherical detonation is a frequent occurrence in reactive gaseous media, which is always accompanied by an explosion. To study the basic laws of spherical detonation, the author used a strong small-volume explosion in a detonating gaseous medium. The model of the transition of strong detonation into the Chapman-Jouguet regime is presented in works [1, 2] and developed on the basis of the point explosion theory. In essence, the transition to normal spherical detonation is the final stage of a point explosion in a reacting gaseous medium, if this is facilitated by the energy potential of the reaction and the physicochemical environmental conditions. The possibility of the stationary regime of spherical detonation follows from the law of conservation of energy and is one of the fundamental results of previous studies [1, 2]. But the study of spherical detonation does not end there. This article discusses other, equally important consequences, resulting from the laws of conservation of energy, momentum and mass. Together, they provide an opportunity to analyze the causes of instability of a normal spherical detonation and an increase in its speed with an unstoppable propagation of a spherical wave in space. In this regard, the task was to study spherical detonation at more remote distances from the center of the explosion. The author set himself the goal of investigating the instability of stationary spherical detonation in gases, the transition of a spherical wave to a plane at infinity, and the energy consequences of such a process. It should be noted

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that the mode of normal spherical detonation is poorly studied in modern gas dynamics, and in the scientific literature is covered only in the works of the author [1-5]. At present, some problems in this field are quite accurately solved by numerical methods [6, 7]. For many researchers, approximation formulas are also a common method for determining the speed of a spherical detonation wave [8, 9]. At considerable distances, when the current front radius is much larger than the critical one ($r \gg R_x$, Figure 1), the Eyring dependence is often used:

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

where r is the current value of the radius of a spherical wave, A is constant, D_n is the velocity of the plane wave, D is the velocity of the spherical wave. Formula (1) indicates the instability of a normal spherical detonation and an increase in its speed in a remote region of propagation, but does not provide information on the causes of this phenomenon.

2. Theoretical Part

2.1. The Change of the Wave Velocity in the Detonating Medium

The author continues to consider a strong explosion of small volume in a detonating gaseous medium and a model for the transition of a blast wave into a wave of normal (stationary) detonation. But if earlier the main attention was paid to the initial stage of this process, that is, the formation of normal spherical detonation, which occurs at a distance of a critical radius R_x from the center of the explosion (Figure 1), then now we will be interested not only in initial, but also in remote distances, when current radius is much larger than critical.

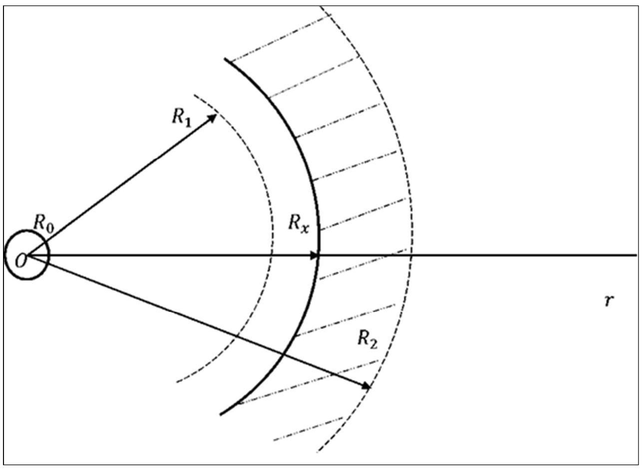

Figure 1. Scenario of continuous transformation of a blast wave into a wave of normal detonation.

Figure 1 shows the radii: R_0 - the radius of the charge, R_x- the initial threshold, R_2- the final threshold for the transition of a strong detonation into the Chapman-Jouguet mode. Using the results of previous studies [1, 2], we present the basic formulas for the velocity of a blast wave at the moment of transition to the Chapman-Jouguet mode:

$$D = \left[\frac{(\gamma+1)^2(\gamma-1)Qc}{4\gamma\mu} + (\xi_0`)^2 \frac{E_0}{\rho_0 r^3} \right]^{\frac{1}{2}} \tag{2}$$

when $r \geq R_1$, where

$$\xi_0` = \left[\frac{3(\gamma-1)(\gamma+1)^2}{16\,\pi\gamma} \right]^{\frac{1}{2}} = const \tag{3}$$

this implies the final formula starting from (2)

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

when $(\xi_0`)^2 \frac{E_0}{\rho_0 r^3} \to 0$ at $r \to R_2$, where $R_2 > R_x \gg R_0$ (Figure 1). In these expressions, the following notation is used: Q - energy of combustion of mole of combustible gas; c - specific coefficient of burnt gas; μ- the molar mass of the mixture; γ- adiabatic index for a given gas mixture; E_0 - the initial explosion energy of a charge of radius R_0; r- current sphere radius; ρ_0–the initial density of the gas mixture before the explosion. The values of the radii R_1, R_x, R_2 are selected based on energy considerations. If $r = R_1$, then $E_0 \gg U$; if $r = R_x$, then $E_0 = U$; when

$r = R_2$ the inequality is fulfilled $E_0 \ll U$, where U is the energy of the burnt gas [10] covered by the blast wave. Formula (4) determines the wave velocity for the stationary mode of spherical detonation

$$D = D_s = const_1 \tag{5}$$

which is called the Chapman-Jouguet regime [11]. In the ideal case [2] such a mode can be established already when $r \to R_x$, where $R_x \gg R_0$. In a real situation, the process of forming stationary detonation stretches in space and time; therefore, to transfer the blast wave to normal spherical detonation, it is necessary to select the transition segment $[R_x; R_2]$, where R_x is the initial and R_2 is a final threshold of such a process (Figure 1).

Let us turn to a graphical representation of the wave velocity as it moves away from the center of the explosion. The system's energy is replenished, so the speed depends not only on the initial energy of the explosion, but also on the burned gas. Considering the transition of the blast wave to the

Chapman-Jouguet regime (Figure 1) and the motion of the wave to infinity, we divide the entire space behind it into three parts: 1) $< R_1$; 2) $R_1 \leq r < R_2$; 3) $r \geq R_2$. In the first area, the energy of the burnt gas is minimal. Only the laws of a point explosion [12] are valid here and the speed of the wave is determined by the initial energy of the explosion E_0 using the formula

$$D = \xi_0{}^{`}\left(\frac{E_0}{\rho_0}\right)^{\frac{1}{2}} r^{-3/2} \quad (6)$$

which is obtained from (2), neglecting the first term of the expression in brackets. The recorded ratio is analogous to the expression of velocity for a point explosion in an inert gas

$$D = \xi_0 \left(\frac{E_0}{\rho_0}\right)^{\frac{1}{2}} r^{-3/2}, \quad (7)$$

where

$$\xi_0 = \left[\frac{3}{4\pi} \times \frac{(\gamma - 1)(\gamma + 1)^2}{3\gamma - 1}\right]^{\frac{1}{2}} \quad (8)$$

For the same values of E_0, formulas (6) and (7) differ only in the coefficients reversed to the variable *r* raised to a fractional power. The plots of the shock wave velocity versus the distance to the center of the explosion are shown schematically in Figure 2 for the two cases mentioned: 1- explosion in a chemically inert gas mixture; 2- explosion in a reacting gas mixture, taking into account the transition of a strong detonation to a stationary one. If we consider the segment $R_1 \leq r < R_2$, then it is more complex, since to determine the velocity in reacting gaseous media, it is necessary to take into account two components of the energy [1, 2].

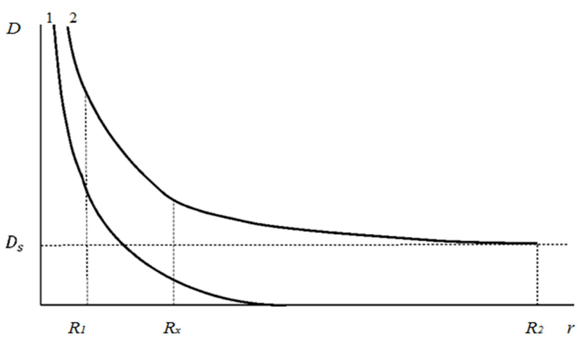

Figure 2. Decrease of the wave velocity with distance from the center of the explosion: 1- explosion in a chemically inert mixture; 2- in a detonating mixture.

$$E = E_0 + U \quad (9)$$

where E_0 is the energy of the explosion, U is the energy of the burnt gas. The wave velocity is calculated from relation (2), which turns into expression (4) as $r \to R_2$. Thus, formula (4) must be applied in the third region, at $r \geq R_2$, when the stationary mode of spherical detonation is established. Here the initial energy of a point explosion does not manifest itself, that is, it is neglected. This part of the space corresponds to the inequality

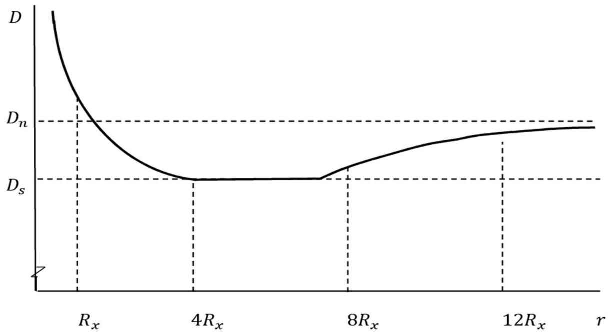

Figure 3. Schematic variation of the speed of a spherical detonation wave with a strong explosion in a detonating gaseous medium.

$E_0 \ll U$, which can be used to find the point R_2 on the number line. The condition is already satisfied when $R_2 \approx (3 \div 4)R_x$, because energy is proportional to the volume and when $R_2 = 3R_x$ it increases by 27 times compared to E_0, and when $R_2 = 4R_x$- by 64 times. In Figure 2 accepted designation $R_2 = 4R_x$. It is logical to ask what happens next, outside the transition zone $[R_x; R_2]$, since the process of propagation of a detonation wave does not stop there, and whether formula (4) is applicable at infinity. Unfortunately, it should be noted that the wave speed increases with increasing charge diameter [8]. There are formulas for approximation and the most well-known of them is the already mentioned Eyring formula. The formula gives approximate results, but they are quite satisfactory. Here it is not the accuracy that is important, but the law according to which the speed of a spherical wave increases at a remote distance (Figure 3). Why this happens we will try to find out a little later, and now we just state the change in the speed of a normal spherical detonation, as well as its ability to go at infinity to a more stable state in the form of a flat stationary detonation. Indeed, as $r \to \infty$, the spherical detonation wave is converted into a plane one, its speed again becomes constant

$$D = D_n = const_2 \quad (10)$$

but the speed value is greater

$$D_n > D_s \quad (11)$$

compared to the previous case (Figure 3).

2.2. Features of Normal Spherical Detonation

The features of stationary spherical detonation follow from the previously proposed model [1, 2] of the transition of a strong detonation to the Chapman-Jouguet regime, which is based on the theory of a point explosion in a reacting gaseous medium. We note only some of them:

1. The formation of a normal spherical detonation begins at a distance R_x from the center of the explosion, when the initial energy of a point explosion becomes equivalent to the energy of the reacted gas swept by the blast wave (Figure 1).
2. In the process of spherical detonation, the energy of the system increases in proportion to the volume of the ball, that is $E \sim r^3$, where $r -$ is the current value of the radius of the sphere, which is the front of the blast wave.
3. The laws of conservation of mass and momentum in a point explosion indicate that the entire mass of gas is collected in a thin layer and moves in the form of a "gas piston", the leading front of which is called the shock wave. A cavity with a minimum amount of reacted substance is formed in the center of the explosion.
4. The law of conservation of energy requires equality of pressures at the front of a spherical detonation wave and behind its front.

Let us stop here for a detailed clarification of the situation. Figure 4 is a pressure diagram for the stationary mode of spherical detonation: P_0 is the pressure ahead of the wave front, P_1 is the pressure at the front, P_c is the pressure behind the front (Jouguet point), d is a segment representing the chemical reaction zone. If the last condition of the listed features is written by the formula

$$P_c = \alpha P_1 \tag{12}$$

where P_c is the pressure behind the wave front, P_1 is the pressure at the front (Figure 4), it will run when

$$\alpha = 1 \tag{13}$$

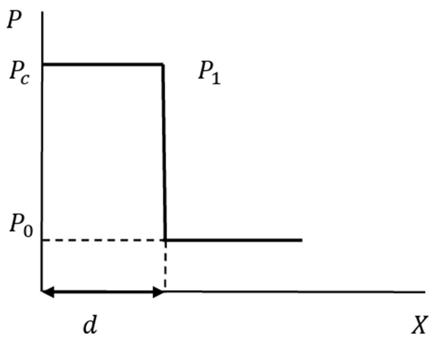

Figure 4. Pressure diagram for the stationary mode of spherical detonation.

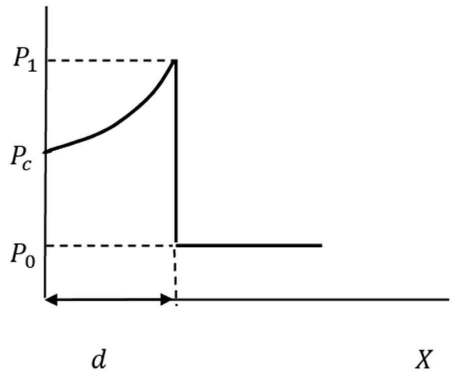

Figure 5. Pressure diagram for stationary flat detonation.

In the case of spherical normal detonation, the energy conservation law [1, 2] gives an unexpected result for α. We see the equality of pressures, the pressure on the inner wall of the "gas piston" (reaction zone) is the same as on the wave front. In classical detonation, where a plane wave is considered, the situation is different, since $\alpha < 1$ Figure 5. To be precise, in the flat stationary detonation regime [13] there are relations

$$P_1 = \frac{2\rho_0 D^2}{\gamma + 1} \tag{14}$$

provided, $M \gg 1$ and

$$P_c = \frac{\rho_0 D^2}{\gamma + 1} \tag{15}$$

when $\frac{P_c}{P_0} \gg 1$, where ρ_0 is the density of the medium ahead of the front, M is the Mach number. From here, using (12), we obtain the real value α for a plane detonation wave,

$$\alpha = \frac{1}{2} \tag{16}$$

Thus, the model of the transition of a blast wave into a detonation wave reveals the specific energy advantages of a normal spherical detonation, which are hidden in the laws of a point explosion and in an optimal spherical wave form. These factors, in particular 3 and 4, contribute to the rapid achievement of the critical temperature necessary to start the reaction. Recall the ideal gas equation. With its help, we obtain the ratio for the temperature in the reaction zone,

$$T_c = \frac{P_c \mu}{\rho_c R} \tag{17}$$

here ρ_c is the density of the medium in the reaction zone (point Jouguet), R is the universal gas constant, μ is the molar mass of the mixture. Analyzing the dependence of temperature on pressure and density at the interface with the reaction products for two cases of detonation (Figure 4, Figure 5), based on the results obtained, it can be argued that there is a higher temperature just behind the spherical wave front. Consequently, in the case of normal spherical detonation, the critical temperature according to (17) is reached faster and easier, with lower energy costs, that is, with lower values of the shock wave velocity. The point explosion model ceases to operate in the transition zone of Figure 1, where R_1 is the initial, and R_2 is a final threshold of such a transition, but the advantages created by a point explosion for normal spherical detonation are retained for a long time due to the geometric waveform. We are talking about the transition of a spherical detonation wave to a plane one at large distances from the center of the explosion. As soon as the relevant parameters P_c and ρ_c in (17) associated with the radius of curvature of the front change, and this is possible already when $r \geq (7 \div 10)R_x$, the speed begins to increase (Figure 3) in order to maintain the temperature in the reaction zone and thereby preserve the detonation process itself. The mechanism of self-regulation, which is always inherent in the detonation process, works, and we see the detonation wave striving to recover lost energy possibilities.

3. Results and Discussion

The transition of a normal spherical detonation to a flat detonation wave is always accompanied by an increase in the speed of the spherical wave. As already mentioned, this is due to a change in the radius of curvature of the front, more precisely, with a change in pressure and density in the chemical reaction zone, which directly depend on the radius. If this phenomenon corresponds to reality, it should manifest itself in any explosive gas mixture to one degree or another. The author carried out calculations to determine the speed of a spherical detonation wave D_s in some detonating gaseous media (Table 1 and Table 2).

Table 1. The detonation velocity and its parameters for a spherical wave in some gaseous media ($P_0 = 1atm$; $T_0 = 293K$).

Gas mixture	γ	Q $[kJ/mol]$	μ $[kg/mol]$	c	D_s $[m/s]$	D_n $[m/s]$	ε [%]
$2H_2 + O_2$	1.4	286.5	0.012	0.66	2550	2830	9.9
$C_2H_2 + 3O_2$	1.37	1299.63	0.0305	0.25	2010	2330	13.7
$CH_4 + 2O_2$	1.35	890.31	0.0266	0.33	1997	2257	11.5
$C_3H_8 + 5O_2$	1.36	2260.4	0.034	0.167	2023	2350	13.9

Table 2. The detonation rate of the hydrogen-oxygen mixture with various impurities ($P_0 = 1atm$; $T_0 = 293K$).

Gas mixture	μ $[kg/mol]$	c	D_s $[m/s]$	D_n $[m/s]$	ε [%]
$(2H_2 + O_2) + O_2$	0.017	0.5	1861	2314	19.6
$(2H_2 + O_2) + 4H_2$	0.0063	0.286	2313	3527	34.4
$(2H_2 + O_2) + N_2$	0.016	0.5	1919	2407	20.3
$(2H_2 + O_2) + 3N_2$	0.02	0.33	1401	2055	31.8

The calculations were carried out using formula (4). The values of the velocity D_n for plane detonation in the corresponding media were taken from the literature [8, 13, 14], where they were determined practically, by measurements. The difference between the submitted speed values is indicated by ε and displayed in percent. The results show that in all cases $D_s < D_n$, and the minimum difference is achieved for the stoichiometric composition of the gas mixture. According to the data in Table 1, ε varies from 9.9% in an explosive hydrogen-oxygen mixture, to 13.9% in a mixture of propane and oxygen. When determining the spherical detonation velocity, the question arises of the exact value of the coefficientγ in formula (4). Note that in deriving this formula, the indicated coefficient is used to find the internal energy of an ideal gas in the reaction zone. It is believed that the adiabatic index is the same, both for the initial state of the mixture before the detonation wave front and for the medium in the reaction zone. This condition is well satisfied for monatomic and diatomic gases. In general, for complex hydrocarbons, the situation is somewhat different. This is a medium filled with radicals and decomposition products of complex compounds that are formed under the action of a shock wave. As a result, for these compounds, the value of the coefficient in the reaction zone may increase by $0{,}01 \div 0{,}02$, approaching the adiabatic index of a diatomic ideal gas [15]. If we take into account this amendment, the difference between D_n and D_s, presented in table 1, will be even smaller. The second important point to which attention should be paid is that the value of the rate of normal spherical detonation in a gaseous medium strongly depends on the heat of combustion of a mole of combustible gas, the molar mass of the mixture and the specific coefficient of the reacted combustible gas. In the case of the same heat of combustion, the result is determined by the ratio between the molar mass and the specific coefficient. For hydrogen-oxygen mixture with various impurities values ε are given in Table 2. With a change in the composition of the mixture and its molar mass, the difference in speed between flat and spherical detonation becomes significant (Table 2), ε increases by two or even three times, compared with initial studies (Table 1).

Analyzing the previous material about the instability of normal spherical detonation and the possibility of the transition of a spherical detonation wave into a plane one, it is important to pay attention to the energy consequences of such a transition. It is necessary to conclude that there are two different stationary states of the detonation phenomenon. The first of them is unstable, here we are talking about normal spherical detonation, the second is sustainable, this is a classic version of flat stationary detonation. If a certain value of the energy of the detonation wave is attributed to each state, then we can speak of two energy levels E_1 and E_2 a stationary detonation (Figure 6). Normal spherical detonation corresponds to a lower energy; we denote it E_1. To study spherical detonation, select a single area (the area is equal to one) on the front surface and direct the velocity vector along the sphere radius from the central part of the selected area. During the transformation of normal spherical detonation into a flat platform remains single, but its energy of motion increases. Let us suppose that the mass of the object under study does not change when changing from one state to another, or changes only slightly, then, based on the results obtained in Tables 1-2, we find the ratio between the energies. Figure 6 feeds a schematic of the energy levels of the stationary detonation regimes of two different hydrogen – oxygen mixtures: E_1, E_2 - respectively, the lower and upper levels for $2H_2 + O_2$; $E_1^`$, $E_2^`$ - for $(2H_2 + O_2) + O_2$.

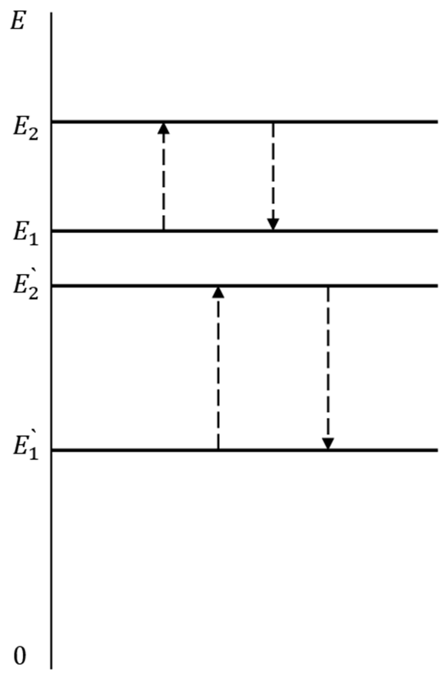

Figure 6. A schematic representation of the energy levels of stationary detonation of different compositions of the hydrogen-oxygen mixture.

In the cases considered in Figure 6.

$$\frac{E_1}{E_2} \approx \frac{D_s^2}{D_n^2} \approx 0{,}81 \tag{18}$$

$$\frac{E_1^`}{E_2^`} \approx 0{,}65 \tag{19}$$

As already noted, the stationary state with energy E_1 is unstable and is easily replaced by a state E_2. The process occurs without authorization, if the energy potential of a chemical reaction allows and consists in the transition of a normal spherical detonation to a flat one, accompanied by an increase in the detonation wave velocity. It is theoretically possible that a detonation breaks down and cannot get to the second level, that is, a change in the waveform is not accompanied by an increase in its speed. Such a wave ceases to be a detonation wave. The “engine” of any detonation wave is a chemical reaction that gives energy to the whole process. If, as a result of a number of reasons, energy ceases to be supplied, or is supplied in insufficient quantity, detonation, slowing down, goes to the lowest energy level, which means that from the stationary state E_2, it again falls into E_1. It can be assumed that a “restart of the engine” occurs here, because spherical normal detonation always has the highest energy potential. Thus, the transition from a lower energy level to a higher one is repeated. This phenomenon is rightly called pulsating detonation and, as we can see, it is simply explained — the transition of a detonation wave from one stationary state to another (shown in Figure 6 by arrows). At the same time, not only the velocity value, but also the geometric shape of the detonation wave front changes periodically. A spherical wave goes into a flat one, and then again into a spherical one. Complex configurations of shock and detonation waves are formed, which is characteristic of pulsating detonation.

4. Conclusions

The work notes the instability of normal spherical detonation at large distances from the center of the explosion. A schematic graph of the speed of a spherical wave, which is initiated by a point explosion in a reacting gas medium, is presented. The graph confirms the findings, including an increase in the wave velocity as it is removed to infinity. The article lists the features of the normal spherical detonation taken from the model of the transition of a blast wave to the Chapman-Jouguet mode. They make it possible to reveal the causes of the instability of the stationary regime for the spherical form of detonation. With specific examples of reacting gaseous media, an increase in the velocity of a spherical detonation wave during the transition to a flat detonation is determined. In each specific case, a quantitative assessment is made of the change in the velocity and energy of the detonation wave. The concept of the energy level for the stationary detonation regime is introduced. The possibility of transition of a normal spherical detonation to a more stable state, with a higher energy level in the form of a flat stationary detonation, is indicated. Thus, it is assumed that there are two energy levels of the stationary detonation regime in gaseous media. The studies conducted by the author prove the existence of an unstable state with a lower level of energy and a stable, in the form of flat classical detonation, with an upper level of energy. This explains the physical nature of the phenomenon of pulsating detonation.

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