DETERMINATION OF DETONATION WAVE VELOCITY IN AN EXPLOSIVE GAS MIXTURE

M.M. POLATAYKO

(180, Grushevskyi Str., Nazavyziv 78425, Nadvirnyanskyi District, Ivano-Frankivsk Region, Ukraine; e-mail: pmm.miron@mail.ru)

PACS 47.40.Rs

The well-known formula for the flat detonation wave velocity derived from the Hugoniót 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.

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

$$\frac{D}{D_n} = 1 - \frac{A}{r} \tag{2}$$

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.

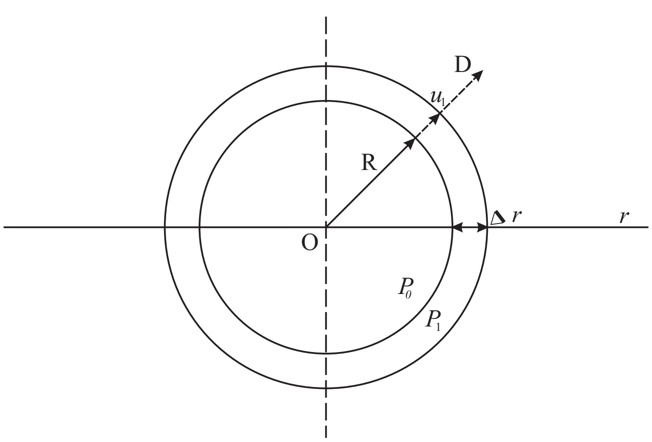

Fig. 1. Schematic diagram of a shock wave from the point explosion

2. 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 consists in the determination of the blast wave velocity, when the wave front is simulated by a rigid piston "jamming" the gas volume located ahead (Fig. 1). The main regularities of the process are well-known [4], 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,

$$\rho_1 = \frac{\gamma+1}{\gamma-1}\rho_0. \tag{3}$$

This formula can be derived from the formula for strong shock waves [5] 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,

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

whence

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

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:

$$u_1 = \frac{2D}{(\gamma+1)\left[1-(c_0/D)^2\right]},$$

where c_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

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

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.

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,

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

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

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

$$\frac{d}{dt}(mu_1) = 4\pi R^2 \alpha P_1,$$

$$0 < R \le R_x^0 E_T + E_k = \text{const},$$

and the condition of strong explosion

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

are valid. Moreover, we have

$$u_1 = \frac{2D}{\gamma+1},$$

and

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

Formula (12) follows from the relation

$$\frac{P_1}{P_0} = \frac{2\gamma M^2 - \gamma + 1}{\gamma+1}$$

of work [5] in the case where $M \gg 1$:

$$\frac{P_1}{P_0} \approx \frac{2\gamma M^2}{\gamma+1} = \frac{2\gamma\,\frac{D^2}{c_0^2}}{\gamma+1} = \frac{2\gamma\,\frac{D^2\rho_0}{\gamma P_0}}{\gamma+1} = \frac{2\rho_0 D^2}{P_0(\gamma+1)},$$

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 $D = dR/dt$ 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

$$D = a\, R^{-3(1-\alpha)} , \tag{15}$$

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

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

so that

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

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

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

Determining the constant a from Eq. (19) 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, Whence, we have

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

Substituting the values of a and α in formula (15), we obtain the formula for the velocity of a blast wave at a point explosion,

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

or

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

where

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

3. 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 to

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

ISSN 2071-0186. Ukr. J. Phys. 2012. Vol. 57, No. 6

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 $R = R_1$ (Fig. 2). Supposing that $E_0 > U$, we determine a condition, under which the detonation energy weakly affects the gas flow [6],

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

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 E_0 is high, and if it is released in a small volume, the flow in the region $R_1 < R_x$ would mainly occur as it does at an ordinary point explosion. On the other hand, for the time moment t_2, at which

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

the combustion processes start to play a dominating role, and the gas flow will possess the main characteristics of the detonation combustion [6].

From the aforesaid, some interesting conclusions can be drawn.

1. The theory of point explosion is applicable 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 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, $E \neq \text{const}$, 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

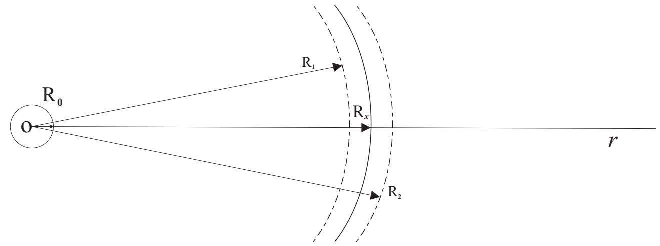

Fig. 2. Scenario of the continuous transformation of a blast wave into a detonation one: R_0 is the charge radius, R_x is the threshold, where the transformation of the strong detonation mode into the Chapman–Jouguet one is possible

of point explosion for a usual non-detonable mixture of gases, it is adopted that $E = \text{const}$, which results in $\alpha = 1/2$. 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:

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

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

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

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

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

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:

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

This result is quite possible, if one takes into account that the energy of the system changes.

4. Results and Their Discussion

Let us determine the shock wave velocity in the critical zone, when $R \to R_x$ (Fig. 2). 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

$$E = V n_{\mathrm{H}_2} q + E_0 \,, \tag{34}$$

where V is the volume of some sphere, n_{H_2} the concentration of hydrogen molecules in this sphere, 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 sphere and the concentration of hydrogen in it are calculated using the known formulas:

$$V = \frac{4}{3}\pi R^3, n_{\mathrm{H}_2} = \frac{P_0}{K^* T_0} N_{\mathrm{A}} c_{\%},$$

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} 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 the molar mass of the mixture. Hence,

$$E = \frac{4}{3}\pi R^3 \frac{P_0}{K^* T_0} N_{\mathrm{A}} c_{\%} q + E_0 \,. \tag{35}$$

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

$$D = \left[\frac{3(\gamma-1)(\gamma+1)^2}{16\pi\gamma}\right]^{1/2} \times$$

$$\times \left[\frac{4/3\pi R^3 \left(\frac{P_0 N_{\mathrm{A}} c_{\%}}{K^* T_0}\right) q + E_0}{\frac{P_0 \mu}{K^* T_0}}\right]^{1/2} \times$$

$$\times R^{-3/2} = \xi_0' \left[\frac{4/3\pi R^3 N_{\mathrm{A}} q c_{\%}}{\mu} + \frac{E_0}{\rho_0}\right]^{1/2} R^{-3/2},$$

where

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

Further transformations give rise to the formula

$$D = \left[\frac{(\gamma+1)^2(\gamma-1)R^{-3}}{4\gamma}\frac{R^3 N_{\mathrm{A}} q c_{\%}}{\mu} + (\xi_0')^2 \frac{E_0 R^{-3}}{\rho_0}\right]^{1/2} =$$

$$= \left[\frac{(\gamma+1)^2(\gamma-1)}{4\gamma}\frac{N_{\mathrm{A}} q c_{\%}}{\mu} + (\xi_0')^2 \frac{E_0}{\rho_0 R^3}\right]^{1/2}.$$

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

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

taking into account that $Q = N_{\mathrm{A}} q$, 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_x, the charge energy E_0 loses its importance; further, the energy of the system is replenished only by the first term, 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 [5, 7]:

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

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 adequate for the description of the continuous process of transformation of the spherical detonation into the plane one. The results of calculations for two different gas mixtures are compared in the Table, where D_s is the velocity of a spherical wave calculated by the new formula (37) at the beginning of the detonation, when $R = R_x$; D_n is the plane wave velocity at the final stage of detonation, when $R \to \infty$, taken from work [8]; 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, formula (37) proves that the mode of normal spherical detonation can

Shock wave velocities

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

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, c_0, i.e. the Mach number M, is often used,

$$M = \frac{D}{c_0}\,. \tag{39}$$

With regard for the formula for the sound velocity

$$c_0 = \sqrt{\gamma\,\frac{P_0}{\rho_0}} = \sqrt{\gamma\,\frac{K^* T_0}{\mu}} \tag{40}$$

and expression (37), we obtain

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

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 initial temperature of the medium T_0. By varying those quantities, it is possible to regulate the shock transition intensity.

5. Conclusion

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.

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 $R \to R_x$ (see Fig. 2 and the model described the transformation of a blast wave in a detonation one). This formula is valid for a bulk spherical wave, in contrast to formula (38) known from the literature, which was obtained for plane waves. The answer to the question about whether or not the detonation will actually take place can be given after studying the kinetics of a chemical reaction at the time moment, when the threshold R_x is passed. 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.

1. S.G. Andreev, A.V. Babkin, and F.A. Baum, *Physics of Explosion* (Fizmatlit, Moscow, 2004) (in Russian).
2. L.P. Orlenko, *Physics of Explosion and Impact* (Fizmatlit, Moscow, 2006) (in Russian).
3. Ch. Mader, *Numerical Modeling of Detonation* (University of California Press, Berkeley, 1979).
4. Ya.B. Zel'dovich and Yu.P. Raizer, *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena* (Dover, New York, 2002).
5. N.N. Sysoev and F.V. Shugaev, *Shock Waves in Gases and Condensed Media* (Moscow State University, Moscow, 1987) (in Russian).
6. V.P. Korobeinikov, *Problems in the Theory of Point Explosions in Gases* (American Mathematical Society, Providence, RI, 1976).
7. W. Fickett, *Introduction to Detonation Theory* (University of California, Berkeley, 1985).
8. G.G. Chernyi, *Gas Dynamics* (CRC Press, Boca Raton, FL, 1994).

Received 15.04.10.
Translated from Russian by O.I. Voitenko

ВИЗНАЧЕННЯ ШВИДКОСТІ ДЕТОНАЦІЙНОЇ ХВИЛІ У ВИБУХОВІЙ ГАЗОВІЙ СУМІШІ

М.М. Полатайко

Р е з ю м е

У науковій літературі загальновідомою є формула швидкості плоскої детонаційної хвилі, що виведена із системи рівнянь Гюгоніо, проте для сферичного реактора користуватися нею важкувато. Метою роботи стало показати можливість втілення положень теорії вибуху в реагуючих газових середовищах для виводу подібної формули, використовуючи спеціальну модель переходу вибухової хвилі в детонацію. Як і в першому, так і в другому випадку діють закони збереження імпульсу, маси і енергії, тому результати мають бути однаковими або майже однаковими, що і підтвердили розрахунки. Таким чином, отримано формулу дуже просту для користування і більш придатну для вивчення граничних процесів об'ємної детонації.