Geometrical shape of the detonation front and instability of the detonation in a round tubek

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Abstract Stability problem is solved analytically for the plane detonation wave propagating in a round tube. Geometrical shape (cell structure) of the detonation front, which is a result of instability development, is substantiated mathematically.

It's known from classical experiments that the detonation waves in explosive gases organize themselves in an unsteady spatial structure (Fig.1.) as a result of instability development. The most interesting regimes are the "spin" (Fig.2) and "gallop", which are typical for detonations of some kinds of mixtures in cylindrical tubes. Those regimes arise probably in mixtures forming unsafe situations in industrial enterprises. Although the processes of the cell forming for the multifront detonations and near-critical regimes are investigated thoroughly in copious experiments and described in literature repeatedly, the full consistent theory for those phenomena is not built yet. The purpose of present work is to analyze mathematically critical regimes of gaseous detonation from the standpoint of the small perturbation theory.
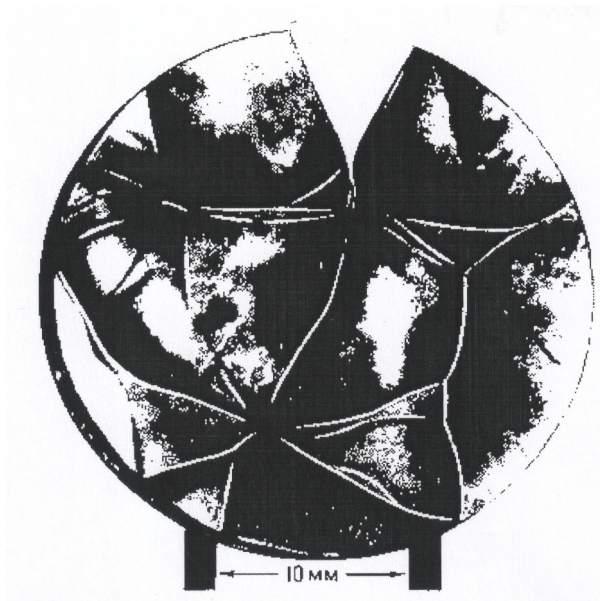
Fig. 1. *A sample of the cellular detonation surface (photograph of the imprints on the sooty tube butt-end; detonation of mixture $2H_2 + O_2$ under initial pressure 300 mm H_g)*

Fig. 2. *Photograph of the single-head ("spin") detonation in gas mixture. Photographing was done through a slot, which was parallel to the tube axis*

The reason for the appearance of the detonation front nonuniformities is the developing of instability of the one-dimensional complex "shock wave – chemical reaction zone", explored experimentally, analytically and numerically. As a result on the non-linear stage the detonation front surface is covered by cells of a characteristic size dependent on the initial pressure and chemical properties of the explosive gas mixture. The numerical and analytical estimates for the mean size of the detonation front nonuniformities were obtained by solving a stability problem of a double-front shock-detonation complex. Thus, distortion of the detonation front and the origin of fractures on it (triple point configurations) was attributed to the two-dimensional instability and the development of the fastest growing perturbations. The method of instability analysis as well as the analysis

of the detonation structure has allowed to take into account the continuous variation of physical and chemical parameters in the course of energy deposition behind a shock front. Moreover, this method has allowed to explain the possible stability of detonation in condensed explosives. However, this stability theory does not account the effect of confinement, whereas in reality the detonation processes occur only in confined volumes. The study of stability and structure of the self-sustaining detonation wave propagating in a cylindrical tube is done by us in [1]. The continuous variation of physical and chemical parameters in the reaction zone behind the shock front is taken into account and essential restrictions are not imposed either by the equation of chemical kinetics or by thermal equation of state both for detonating substance and for the detonation products.

The following mathematical model of a detonation is considered. Along a z-axis, at $z < 0$ the inviscid gas moves at a stationary supersonic velocity. Plane $z = 0$ corresponds to a shock wave. In the zone $0 \leq z \leq L$ chemical transformations occur while zone $z > L$ is occupied by the detonation products. Physical parameters of explosive mixture, gas in the chemical transformation zone and detonation products are related to each other by the conservation laws of mass, momentum, and energy. Chemical reaction is assumed to be governed by a single variable, unburnt mass fraction or progress variable, β. At the shock front, $\beta = 1$. At termination of chemical reaction, i.e., at $z = L$, $\beta = \beta_2$ ($0 \leq \beta_2 < 1$). At $\beta = \beta_2$ the flow velocity is equal to the local speed of sound (Chapman-Jouget condition).

At $z > 0$ the flow field is governed by a set of gasdynamic equations and equation of chemical kinetics:

$$
\begin{cases}
\frac{d\rho}{dt} + \rho \, div \, \overrightarrow{u} = 0, \\
\rho \frac{d\overrightarrow{u}}{dt} + \overrightarrow{grad} p = 0, \\
\frac{\partial}{\partial t}\left(pE + \frac{\rho u^2}{2} \right) + div\left[\overrightarrow{u}\left(\rho E + p + \frac{\rho u^2}{2} \right) \right] = 0, \\
\frac{d\beta}{dt} = f(\beta, p, \rho),
\end{cases}
\tag{1}
$$

where $\overrightarrow{u}$ is the velocity vector, $u^2 = \overrightarrow{u}^2$, ρ is the density, is the pressure, is the specific internal energy, and

$$
E = e + \beta Q,
\tag{2}
$$

Q is the chemical energy source per unit mass of gas and $e = e(p, \rho)$. For the thermally perfect gas:

$$
e = \frac{1}{\gamma - 1} \frac{p}{\rho} + const,
\tag{3}
$$

where γ is the ratio of thermal specific heats.

Function f in the equation of chemical kinetics is assumed to be sufficiently smooth (as well as function $e\,(p, \rho)$, expressing the thermal equation of state). The explosive gas flows in a round cylindrical tube of radius r_0, therefore Eqs. (1) should be formulated in a cylindrical frame of reference.

Let us investigate the stability of the basic solution of Eqs. (1) in relation to small perturbations u'_{jr}, $u'_{j\varphi}$, u'_{jz}, ρ'_j, p'_j, β'_j corresponding to radial, tangential and axial components of a velocity vector, pressure, density and progress variable, in the reaction zone ($j = 1$) or in the detonation products ($j = 2$), assuming that $\beta'_2 = 0$. As a result the following linearized equations can be obtained from Eqs. (1):

$$
\begin{cases}
\dfrac{\partial \rho'_j}{\partial t} + \dfrac{\partial}{\partial z}\left(\rho u'_{jz} + u_j \rho'_j \right) + \dfrac{\rho_j}{r}\left[\dfrac{\partial (r u'_{jr})}{\partial r} + \dfrac{\partial u'_{j\varphi}}{\partial \varphi} \right] = 0, \\[2mm]
\dfrac{\partial u'_{jr}}{\partial t} + u_j \dfrac{\partial u'_{jr}}{\partial z} + \dfrac{1}{\rho_j}\dfrac{\partial p'_j}{\partial r} = 0, \\[2mm]
\dfrac{\partial u'_{j\varphi}}{\partial t} + u_j \dfrac{\partial u'_{j\varphi}}{\partial z} + \dfrac{1}{\rho_j r}\dfrac{\partial p_j}{\partial \varphi} = 0, \\[2mm]
\dfrac{\partial u'_{jz}}{\partial t} + \dfrac{\partial}{\partial z}\left(u_j u'_{jz} \right) + \dfrac{1}{\rho_j}\dfrac{\partial p'_j}{\partial z} - \dfrac{1}{\rho_j^2}\dfrac{dp_j}{dz}\rho'_j = 0, \\[2mm]
\rho_j\left(\dfrac{\partial \beta'}{\partial t} + u_j \dfrac{\partial \beta'}{\partial z} \right) + u_j \dfrac{d\beta}{dz}\rho'_j + \dfrac{\partial p'_j}{\partial t} + \dfrac{1}{Q(\gamma_j-1)}\dfrac{\partial p'_j}{\partial t} + \dfrac{u_j}{Q(\gamma_j-1)}\dfrac{\partial p'_j}{\partial z} + \\[2mm]
+ \dfrac{j_j}{Q(\gamma_j-1)}\dfrac{du_j}{dz}p'_j - \dfrac{j_j p_j}{\rho Q(\gamma_j-1)}\left(\dfrac{\partial \rho'_j}{\partial t} + u_j \dfrac{\partial \rho'_j}{\partial z} + \dfrac{du_j}{dz}\rho'_j \right) = 0, \\[2mm]
\dfrac{\partial \beta'}{\partial t} + u_j \dfrac{\partial \beta'}{\partial z} + \dfrac{d\beta}{dz}u'_{jz} - u_j \dfrac{d\beta}{dz}\left(\dfrac{\partial f}{\partial \beta}\beta'_j + \dfrac{\partial f}{\partial p_j}p'_j + \dfrac{\partial f}{\partial \rho_j}\rho'_j \right) = 0,
\end{cases} \tag{4}
$$

where

$$
\gamma_j = 1 + \left[\left(\dfrac{\partial e_j}{\partial p_j} \right)_{\rho j} \rho_j \right]. \tag{5}
$$

In the particular case of thermally perfect gas, γ_j is the ratio of specific heats. The solutions of Eqs. (4) should obey to the condition:

$$
u'_{jr}\,|_{r=r_0} = 0, \tag{6}
$$

and the condition of regularity at $r \to 0$. In view of it, the solution is taken in the form

$$
\begin{aligned}
\dfrac{u'_{jz}}{u_2} &= y_{1j}(z)F(r, \varphi, t); \\[1mm]
\dfrac{u'_{jr}}{u_2} &= y_{2j}(z)r_0 \xi_{nk}^{-1} \dfrac{d}{dr} \ln J_n\big(\xi_{nk} r r_0^{-1} \big) F(r, \varphi, t); \\[1mm]
\dfrac{u'_{j\varphi}}{u_2} &= y_{3j}(z) r r_0^{-1} \xi_{nk}^{-1} n F(r, \varphi, t); \\[1mm]
\dfrac{p'_j}{p_2} &= y_{4j}(z)F(r, \varphi, t); \\[1mm]
\dfrac{\rho'_j}{\rho_2} &= y_{5j}(z)F(r, \varphi, t); \\[1mm]
\beta' &= y_{6j}(z)F(r, \varphi, t),
\end{aligned} \tag{7}
$$

where

$$F(r, \varphi, t) = exp\left(\omega r_0^{-1} u_2 t + in\varphi\right) J_n\left(\xi_{nk} r r_0^{-1}\right), \qquad (8)$$

and ω — a complex value (dimensionless eigenvalue), n is the azimuthal wave number $(n = 0, 1, 2, \ldots)$, $J_n(\xi)$ is the cylindrical functions of the 1-st kind of order n, ξ_{nk} is the k th root of the equation $dJ_n(\xi)/d\xi = 0$, y_{jk} $(k = 1, ..., 5)$ — dimensionless function of z.

For the Chapman-Jouget detonation $(u_2 = a_2$, i.e. $M_2 = 1$, where $M_2 = \frac{u_2}{a_2}$ is the Mach number, $_2$ is the speed of sound in the detonation products) the functions $y_{2k}(k = 1, ..., 4)$ are determined to be the solutions of system of the linear homogeneous differential equations with constant coefficients and contain three uncertain constants $A_{2l}(1, 2, 3)$.

The equations of the perturbed shock front and the surface of chemical reaction termination are set as

$$z = \varepsilon_1(r, \varphi, t), \quad z = L + \varepsilon_2(r, \varphi, t), \qquad (9)$$

where

$$\varepsilon_j = A_{0j} r_0 F(, \varphi, t). \qquad (10)$$

In the linear approximation, the laws of conservation of mass, momentum, energy and unburnt mass fraction at the shock front $(z = 0)$ are given by

$$
\begin{aligned}
&u_1 \rho_1' + \rho_1 u_{1z}' = \left(\rho_1 - \rho_0\right)\frac{\partial \varepsilon_1}{\partial t}, \\
&u_{1r}' = \left(u_0 - u_1\right)\frac{\partial \varepsilon_1}{\partial r}, \\
&u_{1\varphi}' = \frac{1}{r}\left(u_0 - u_1\right)\frac{\partial \varepsilon_1}{\partial \varphi}, \\
&p_1' + u_1^2 \rho_1' + 2\rho_1 u_1 u_{1z}' = 0, \\
&[(\gamma_1 - 1)\rho_1 - (\gamma_0 + 1)\rho_0]p_1' + \left[(\gamma_1 - 1)p_1 + (\gamma_0 + 1)p_0\right] + \\
&+\lfloor \rho_1' + 2(\gamma_1 - 1)Q_{\rho_1}^2 \beta' \rfloor = 0, \\
&\beta' + \varepsilon_1 \frac{d\beta}{dz} = 0,
\end{aligned}
\qquad (11)
$$

where index 0 denotes parameters of a unperturbed stream at $z < 0$.

As the perturbations behind shock front are continuous everywhere along the tube, the requirements of a continuity of all parameters at the perturbed surface of the chemical reaction termination should be used.

After simple transformations one arrives at the following boundary value problem:

$$
\begin{aligned}
&\overrightarrow{R}(0) = \overrightarrow{R}_0, \\
&\overrightarrow{R}(1) = \overrightarrow{R}_m, \\
&\frac{d\overrightarrow{R}}{d\widetilde{z}} = G(\widetilde{z})\overrightarrow{R},
\end{aligned}
\qquad (12)
$$

with

$$\overrightarrow{R}(0) = A_{10}\left(\overrightarrow{R}_0^{(1)} + \omega \overrightarrow{R}_0^{(2)}\right), \tag{13}$$

$$\overrightarrow{R}(m) = \Sigma_{R=0}^3 A_{2l} \overrightarrow{R}_m^{(l)}, \tag{14}$$

$$G(\widetilde{z}) = G^{(1)}(\widetilde{z}) + \omega G^{(2)}(\widetilde{z}), \tag{15}$$

$$\widetilde{z} = \frac{z}{L}, \tag{16}$$

$$\overrightarrow{R} = \begin{pmatrix} y_{11} \\ y_{12} \\ y_{13} \\ y_{14} \\ y_{15} \end{pmatrix}, \tag{17}$$

where G is the 5×5 matrix.

It is rather difficult to find a precise solution of the system of ordinary linear homogeneous differential equations with variable coefficients. Therefore, the boundary value problem (13) is solved approximately [1] by the Euler method. As a result, one arrives at the equation for definition of eigenvalues

$$F(\omega) = 0, \tag{18}$$

where function $F(\omega)$ represents a polynomial of $m+5$ order, where m the number of intervals in Euler method. If this equation has a solution with a positive real part, it is evidence of the detonation wave instability. The eigenvalue ω is, in general, the complex function of parameter ξ_{nk}.

Calculating of the pulsation structure of detonation waves is based on the discrete spectrum of values ξ_{nk} satisfying a boundary condition (6), it is possible to choose the eigenvalues ω (ξ_{nk}), providing the fastest growth rate of perturbation amplitude, and therefore the maximal distortion of the front. ξ_{nl} value corresponds these eigenvalues almost always. Thus it is possible to calculate the mean size of nonuniformities (cells) in the detonation wave propagating in an explosive gas. Particular calculations were performed for mixtures $2H_2 + O_2 + 7Ar$ and $2H_2 + O_2 + 7$. He with the kinetics of [2] and are compared to results of experiments [3] - [5] and numerical analysis [2], [6]. The agreements between the present analysis and experimental data can be treated as satisfactory.

For the formation of the detonation structure, parameter

$$\delta = Lr_0^{-1}, \tag{19}$$

which shows the ratio of the reaction zone width to the tube radius is the most important one. Increase of the tube radius r_0 or decrease of the reaction zone

width L (that is possible, for example, when the explosive gas pressure $_0$ increases or the inert additions) leads to decrease of δ.

For the thermally perfect gas with the model kinetics [2] if $\delta \geq 0.5$ the instability takes place only for $n = 0$. But in this case $\xi_{01} = 0$, and it contradicts (7), and the case, corresponding to $\xi_{02} = 3.83$ is realised. Absence of the dependance of perturbations from φ means, that gas produces radial acoustic oscillations. But under $n = 0$, $\xi_{01} = 0$ it is necessary to go over to another (one-dimensional) stability problem. This problem is solved by us before [1] and the instability of the gaseous detonations to the one-dimensional perturbations is proved. Developing of such instability may be accepted for theoretical explanation of the galloping detonation regime [5]. At the non-linear stage of developing one-dimensional (axial) and radial perturbations will interact. The result of such interaction is non-one-dimensional character of the detonation "gallop", that is observed in experiments [5].

If $0.3 \leq \delta \leq 0.5$ instability develops under $n = 1$, $\xi_{11} = 1.84$, which corresponds to the single-head spinning detonation (Fig.2) [4], [5]. If $0.1 \leq \delta \leq 0.3$ instability develops under $n = 2$, $\xi_{21} = 3.05$, which corresponds to the double-head spinning detonation [4], [5]. And so on, as δ decreases, n increases, that means existence of the multi-head spin, i.e. cell structure of detonation (Fig.1).

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