Model of non-ideal detonation of condensed high explosives

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Abstract. The Zeldovich–Neumann–Doering theory of ideal detonation allows one to describe
adequately the detonation of charges with near-critical diameter. For smaller diameters,
detonation velocity can differ significantly from an ideal value expected based on equilibrium
chemical thermodynamics. This difference is quite evident when using non-ideal explosives;
in certain cases, this value can be up to one third of ideal detonation velocity. Numerical
simulation of these systems is a very labor-consuming process because one needs to compute
the states inside the chemical reaction zone, as well as to obtain data on the equation of state of
high-explosive detonation products mixture and on the velocity of chemical reaction; however,
these characteristics are poorly studied today. For practical purposes, one can use the detonation
shock dynamics model based on interrelation between local velocity of the front and its local
curvature. This interrelation depends on both the equation of state of explosion products, and
the reaction velocity; but the explicit definition of these characteristics is not needed. In this
paper, experimental results are analyzed. They demonstrate interrelation between the local
curvature of detonation front and the detonation velocity. Equation of detonation front shape
is found. This equation allows us to predict detonation velocity and shape of detonation wave
front in arbitrary geometry by integrating ordinary differential equation for the front shape with
a boundary condition at the charge edge. The results confirm that the model of detonation shock
dynamics can be used to describe detonation processes in non-ideal explosives.

The theory of ideal detonation adequately describes detonation of charges with diameter,
which is close to ultimate. With smaller diameters, the detonation velocity may sufficiently differ
from ideal value, which is expected on the basis of equilibrium chemical thermodynamics. This
difference is widely developed for insensitive high explosives and in separate cases, may achieve
up to 30% of ideal detonation velocity [1]. This is related to the fact that under detonation
of the charges with finite diameters, detonation front cannot be flat. Actually due to limited
character of chemical transformation velocity directly behind the flat front of detonation wave
(DW), the flow is subsonic. That is why, lateral unloading waves that appear under compressed
matter expansion to the sides, penetrate primary the front, decreasing pressure on it and thereby
decreasing its velocity, first of all near the charge. Thus shock front of detonation wave gets
a shape that is protuberant towards the detonation propagation, and after completion of some
section of development, it gets stationary shape.

Numerical modeling of such systems is rather labor intensive, as far as it is necessary to
calculate the states inside chemical reaction zone and it is also necessary to have information
on equations of state for a mixture of the high explosive (HE) and explosion products (EP) and
chemical reaction velocity that currently are studied poorly. For practical purposes, we can use a model of “detonation shock dynamics” (DSD), which is based on interconnection of local front velocity with local curvature of detonation front. The interconnection depends on both equation of state for EP mixture and reaction velocity, but it is not necessary to explicitly specify these characteristics.

The work analyzes the results of experiments that demonstrate the interconnection of local curvature of detonation wave front with the value of detonation velocity for this section of front. Experimental investigation into the process of detonation wave development and propagation in cyclic samples out of low-sensitivity HE was performed in the range of diameter change (1–10) $d_{cr}$ ($d_{cr}$—critical diameter of detonation). Initiation was made by a flat and divergent wave. The scheme of experiments is shown in figure 1. Streak camera recorded time profiles of detonation wave arrival to the edge surface of investigated cylindrical samples, which were recalculated into the profiles of detonation waves with regard for the velocity. Detonation velocity was registered by electro-contact technique.

During experiments, we determined the profiles of detonation wave front at the section of development [2,3] and after detonation establishment [2,3] in cylindrical samples with diameter 15, 20, 40, 60 and 120 mm, as well as the values of detonation velocity corresponding to them. Determination of the shape and velocity in the process of detonation development is demonstrated by the results (figure 2) of measuring the velocity by electro-contact gauges that are installed at various removal $r$ (figure 1) from the axis of cylindrical charge. Diameter of HE samples was 120 mm. Initiation was made by a flat wave. Electro-contact gauges were installed on the axis and at a distance 20 and 40 mm from the axis. The results in figure 2 show that the velocity of each section of the front in the process of detonation development is different. The character of the velocity change for different front sections also differs. The gauges installed on the axis of cylindrical part ($r = 0$ mm) show the establishment of a flat detonation wave [2,3], when the velocity passes via maximum value corresponding to $\sim 1.01D_{st}$. The gauges shifted from the axis to the periphery of the charge demonstrate the character of detonation establishment, which is observed with initiation of divergent wave [2,3]. Such character of the velocity change for various sections of the front is explained by the curvature of the latter under the impact of lateral rarefaction waves.

In the course of investigations, it was established that the character of detonation development does not depend on HE charge diameter. This is confirmed by the data obtained under flat-
wave initiation of cylindrical parts with diameter 60 and 120 mm that are shown in figure 3. The results on the plot are given in relative detonation velocity of cylindrical HE charges, as a function of the ratio of charge length to its diameter.

The results given in figure 3 show that, in the beginning, detonation velocity rapidly increases with the charge length $x$, achieving at $x \approx d/2$ the value of stationary detonation velocity for this charge diameter $D_{st}(d)$. At $x \approx 1.5d$, detonation velocity achieves its maximum value exceeding $D_{st}(d)$ by $\sim 1\%$. After that, the lateral loading gradually decreases the detonation velocity, and at the charge length higher than $3d$, the detonation velocity is practically equal to $D_{st}$.

After passing the section of development, which is as a rule of $3d$ ($d$—charge diameter), detonation velocity and shape are established, and in further, for this diameter, remain constant [2, 3]. In order to determine the front curvature, the obtained profiles were approximated by analytical dependence of the following form:

$$z = f(z),$$

where $r$—radial coordinate, which is measured from the charge axis, $z$—axial coordinate, which is calculated from the point of the detonation wave front arrival to the charge edge (figure 2).

The curvature of any three-dimensional surface is determined from corresponding combination of its first and second spatial derivatives by orthogonal directions [4]. The first main curvature by radial coordinate is expressed as follows:

$$k_1(r) = \frac{z''(r)}{[1 + z'(r)^2]^{3/2}}.$$  

In this charge geometry, it is assumed that the profile of detonation wave front is symmetrical relatively to the axis, and this permits to express the second main curvature:

$$k_2(r) = \frac{\sin \theta}{r} = \frac{\sin \arctan(z'(r))}{r} = \frac{z'(r)}{r[1 + z'(r)^2]^{1/2}}.$$  

**Figure 2.** Detonation development in high-explosive charge of 120-mm diameter under flat-wave initiation.
Figure 3. Detonation development under flat-wave initiation of parts with diameter of 60 and 120 mm.

Figure 4. Scheme of established detonation in cylindrical HE charge.

For average surface curvature, we can write

\[ k(r) = \frac{1}{2} \left( \frac{z''(r)}{[1 + z'(r)^2]^{3/2}} + \frac{z'(r)}{r[1 + z'(r)^2]^{1/2}} \right). \]  (4)
Obtained equation is differential equation of the second order. Specifying the concrete type of
dependence \( k(D) \), it is possible to get analytical solution for this equation. The authors of [1,5,6]
got approximated solution for this equation in the form of logarithm of Bessel function:
\[
z(r) = \ln(J_0(r)),
\]
where \( J_0(r) \)—Bessel function of the first kind, which for differencing convenience with accuracy
up to a constant, may be expressed via trigonometric functions. Finally, for the function \( z(r) \),
the following expression was proposed:
\[
z(r) = -\sum_{i=1}^{n} a_i \left( \ln \left( \cos \left( \eta \frac{\pi r}{2R} \right) \right) \right)^i,
\]
where \( r \)—radial coordinate; \( R \)—radius of cylindrical charge; \( a_i, \eta \)—adjustable coefficients.

Experimentally obtained image of detonation wave front was digitized with resolution by
radial coordinate \( \Delta r = 0.07 \text{ mm} \). After that, obtained profile (figure 5) was processed
by analytical dependence (5) adding free term into it, which was to include possible front asymmetry.

Unlike investigators [1,6], who used three first elements of series (6), in this work, the number
of series terms was increased up to five, that permitted to expand the range of this function.
The results of processing are shown in Figure 5. The same figure shows deviations of experimental data from approximating function. Deviation between experimental and calculated values, except the edge zone, does not exceed 0.05 mm, with recalculation for times, it gives the value $\sim 0.007 \mu s$.

After substituting the coefficients, which were determined as the result of approximation, in expression (9), and in analytical expressions for the first and second derivatives of function $z(r)$ with regard for formula (6), the function $k(r)$ of DW front curvature was determined.

From Figure 4, it is seen that normal component of detonation velocity along radial coordinate $r$ is related to stationary detonation velocity for this diameter $D_{st}$ (in cylindrical geometry) in the following way:

$$D_n(r) = D_{st} \cos \theta(r) = D_{st} \cos \arctan(z'(r)) = \frac{D_{st}}{[1 + (z'(r))^2]^{1/2}},$$

where $\theta(r)$—angle between normal component of detonation velocity vector and axis of the charge by radial coordinate.

Obtained are two functions $D_n(r)$ and $k(r)$ in parametric form give connection of normal component of detonation velocity with curvature along DW profile (Figure 6). Dependence $D_n(k)$, which is the connection of normal component of detonation velocity with curvature along radial coordinate, is in good agreement with the data that were obtained earlier for various diameters [2, 3].

Theory of DSD assumes that normal detonation velocity $D$ is determined by a full front curvature $k$, and that edge angle $\theta$ (angle between front normal and HE edge) is unique for each combination of HE and lining material. Using this model, we can obtain conventional equations that describe stationary two-dimensional profiles of detonation profile in HE charges, having the shape of a plate, cylinder and a ring.
Let us consider detonation of HE cylinder lined by inert material, which is detonated in stationary regime and detonation velocity in the center is $D_{st}$. For normal component of detonation velocity, we can write

$$D_n(k) = \frac{D_{st}}{\sqrt{1 + (z'(r))^2}},$$

(8)

where function $z(r)$ describes the front profile, and $r$—radius. According to (4) expression for the full front curvature will be written as follows:

$$\frac{1}{2} \left( \frac{z''(r)}{[1 + z'(r)^2]^{3/2}} + \frac{z'(r)}{r[1 + z'(r)^2]^{1/2}} \right) = k \frac{D_{st}}{\sqrt{1 + (z'(r))^2}}.$$

(9)

Substituting $y = z(r)'$ and transformation give

$$\frac{dr}{dy} = \left( 2k \frac{D_{st}}{\sqrt{1 + y^2}} - \frac{y}{r\sqrt{1 + y^2}} \right)^{-1} \left( 1 + y^2 \right)^{-3/2},$$

(10)

$$\frac{dz}{dy} = \left( \frac{2}{y} k \frac{D_{st}}{\sqrt{1 + y^2}} - \frac{y}{r\sqrt{1 + y^2}} \right)^{-1} \left( 1 + y^2 \right)^{-3/2}.$$

(11)

Integrating of equations (10), (11) gives the profile of stationary detonation front $z(r)$ for specified $D_{st}$. Initial point is $y = 0, r = 0, z = 0$, and finite point is $y = \tan(\theta)$. Thus $D_{st}$ definitely determines the profile of stationary detonation front $z(r)$, which corresponds to several combinations of the cylinder radius $R_0$ and lining material (edge angle $\theta$).

Therefore, we got conventional differential equations those describe the profiles of stationary two-dimensional detonation fronts in HE cylinder. It was revealed that one and the same stationary profile of detonation front corresponds to several combinations of lining material and determining charge size. Equation for the shape of detonation wave front permits to predict detonation velocity and the shape of wave front in arbitrary geometry by integrating conventional differential equation with boundary condition in the form of angle $\theta$ on the charge boundary.

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