CALCULATING THE STRUCTURE OF DETONATION WAVES

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Some results of calculations are shown which have been obtained for detonation waves with the fission of the explosive material occurring at a finite rate.

When a detonation wave produced by a charge of explosive material propagates, then, according to the hydrodynamic theory of Zel'dovich [1], there appears at the wave front a distinct high-pressure (chemical) zone. This zone, within which the release of energy essentially occurs, is assumed to be stationary under the steady-state condition of self-sustaining detonations and to be terminating into the Jouget mode. The Jouget mode constitutes the front of a following rarefaction wave, whose profile is determined either by the exhaust of the explosion products at the tail end in the case of a one-dimensional detonation, or by the combined effect of explosion products expansion from the lateral and from the tail surface of the charge if the charge has a finite diameter.

An approximate expression for the width of the chemical zone was derived by Zel'dovich and Kompaneets [2]. For common explosive materials the dimensions of this zone do not exceed 0.1-1.0 mm [3]. As the detonation wave travels a sufficiently long distance, many times exceeding the width of the chemical zone, it appears possible to disregard in this analysis the chemical zone and to consider the Jouget mode as the wave front. In this case the solution will be a self-simulating one and relatively simple to arrive at, if the isentropy of the explosion products expansion is known. With various assumptions regarding the isentropy of the explosion products, such solutions were obtained for planar and for spherically propagating detonation waves [4].

Most methods of calculating detonation waves (e.g., [5]) do not convey the structure of these waves; in particular, they do not describe the chemical zone.

There are many problems at hand, however, where the structure of the chemical zone must be known and, consequently, their solution should take into account the kinetics of the chemical reactions. One-dimensional problems of this kind include initiating the explosive material with a shock wave, determining the detonation transient, and many others.

One important problem is to determine the critical diameter of the explosive charge. A general concept about the physical significance of this diameter was developed by Khariton; approximate solutions were given in subsequent works (e.g. [6]).

The problem is made more complicated by having the kinetics of energy release behind the detonation wave front entered into the calculations, and a sufficiently complete solution can be obtained only with the aid of a computer. Calculations for one-dimensional waves [7, 8, 9] and for two-dimensional flow [10, 11] have shown that this method is promising for the study of unstable detonations.

In this article we present the results of calculations made for detonation waves according to the Sigma program [12] and with the simplest assumptions regarding the equations of state for the medium as well as the equations of fission kinetics for the explosive material. The study covered the detonation build-up after a short intensive pulse and the termination of the detonation wave into the stationary mode. Some of the calculations were made for cylindrical charges of explosive material with a finite diameter, in order to explain the effect which the lateral exhaust of the explosion products has on the detonation wave structure and in order to determine the limiting conditions for the occurrence of detonations.

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The quantities involved here are given in the following units: time in μsec, distance in mm, density in g/cm^3, specific energy in 10^{10} erg/g, velocity in 10^5 cm/sec, and pressure in 10^{10} dyne/cm^2.

1. The motion of a compressible gas in which monomolecular and bimolecular chemical reactions take place is described by the following system of equations:

$$\frac{d\rho}{dt} + \rho \operatorname{div} U = 0, \qquad \rho \frac{dU}{dt} + \operatorname{grad} p = 0 \tag{1.1}$$

$$\frac{dE}{dt} + p \frac{d}{dt} \frac{1}{\rho} = \sum_{k=0}^{N} c_{0k} L_k, \qquad p = p(\rho, E) \tag{1.2}$$

$$\frac{da_\mu}{dt} = \sum_{k=1}^{N} c_{\mu k} L_k, \quad L_k = s_{k\mu\nu} a_\mu a_\nu \rho \quad (s_{k\mu\nu} = s_{k\mu\nu}(\rho, E)) \quad \begin{pmatrix} \mu, \nu = 1, \ldots, n \\ k = 1, \ldots, N \end{pmatrix} \tag{1.3}$$

Here ρ, U, p, and E are, respectively, the density, the velocity, the pressure, and the specific internal energy of the substance; a_μ is the "mass" concentration of the μ-th substance, i.e., the ratio of the mass of a given substance to the total mass of the mixture; $c_{\mu k}$ is the efficacy of the k-th reaction with respect to the μ-th substance; $s_{k\mu\nu}$ is the rate of interreaction between the substances μ and ν; n is the number of substances; N is the number of reactions; c_{0k} is the heat content in the k-th reaction; and the symbol

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (U\nabla)$$

designates the "material derivative." In order to yield a numerical solution to the system (1.1), (1.2), (1.3), the calculations were based on the method of separating the physical processes. For each computation step corresponding to certain instant of time the motion of an "inert" (nonreacting) gas was calculated first, i.e., Eqs. (1.1) and (1.2) were solved with the term corresponding to the release of energy omitted in (1.2). Changes in the concentrations of substances and in the densities of internal energy due to chemical reactions were calculated next (a substance assumed here to be motionless), i.e., the system of ordinary differential equations (1.2), (1.3) was solved next. At this stage of the computation, the second term on the left-hand side of (1.2) was omitted. That concluded the calculations for a given step in the procedure.

The system of gas-dynamics equations was solved by the method shown in [12]. In solving this system of equations with a sliding numerical grid there arises the problem of transposing (interpolating) the values onto a new grid. The mass concentrations of substances were transposed onto a new grid with the Law of Mass Conservation observed for each component of the mixture, i.e., according to the same rules as those applied to the densities of internal energy.

The system (1.2), (1.3) was solved by the method shown in [13]. Reaction cycles are set up for each computation point. The number of reaction events is determined by

$$L_k = \frac{s_{k\mu\nu} a_\mu a_\nu \rho}{1 - \tau\rho s_{k\mu\nu} (a_\mu b_{\nu k} + a_\nu b_{\mu k})}, \qquad b_{\mu k} = \begin{cases} c_{\mu k} & (c_{\mu k} < 0) \\ 0 & (c_{\mu k} \geqslant 0) \end{cases} \tag{1.4}$$

Here a_μ is the concentration of the μ-th substance before the k-th reaction is counted, and τ is the interval of integration with respect to time. One then recalculates the internal energy

$$E^{n+1} = E^n + \tau c_{0k} L_k \tag{1.5}$$

and the concentration

$$a_\nu^{\,n+1} = a_\nu^{\,n} + \tau c_{\nu k} L_k \tag{1.6}$$

of substances participating (reagents and products) in a given reaction.

This computation scheme is of first-order accuracy; it meets the requirements of equilibrium and monotonicity. It can be shown that with such a computation schedule the concentrations will never be negative. Consequently, the computation step or the time interval with respect to which integrations in (1.2), (1.3) are performed may be chosen quite large: the same as the integration interval in the system of gas-dynamics equations.

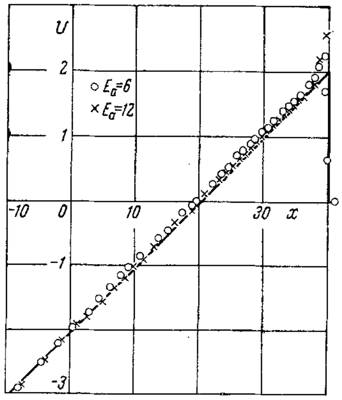

Fig. 1

2. The application of dynamic methods for studying the properties of substances at high pressures [14] made it possible to obtain sufficiently reliable information concerning the equations of state for both the explosive material and the explosion products within the detonation range. A detailed interpretation of accumulated experimental data would require a formulation of rather complex equations of state [15]. On the other hand, the kinetics of chemical reactions behind the detonation wave front has not been investigated. The Arrhenius relation is used for the rate of chemical reactions in practically all references [7, 10, 11]. It will be used also in this article.

In order to facilitate the calculations, a qualitative concept of the detonation buildup has been developed: in accordance with the simplified representation of the detonation kinetics, the simplest equation of state for an ideal gas was used for the explosion material and for the explosion products; the relation $p = p(\rho, E)$ was put in the form

$$p = (\gamma - 1)\rho E$$

If $E = c_V T$, then the equations of the fission kinetics for an explosive material (1.2), (1.3) can be written as

$$\frac{da}{dt} = -\nu a\rho \exp\left(\frac{-E_a}{E}\right) = -L, \qquad \frac{dE}{dt} = qL \tag{2.1}$$

Here a is the concentration of the explosive material, E_a is the activation energy, and q is the heat content of the explosive material.

The value $\gamma = 3$ was assumed in the equation of state, in order to obtain at the detonation front a compression ratio usually realized with compact explosive materials.

The first series of calculations dealt with the termination of a planar detonation wave into the classical mode, which corresponds to an instantaneous release of energy behind the shock front. This was taken care of in the calculations by an appropriate choice of values for v and E_a in Eq. (2.1). In Fig. 1 is shown the (U, x) profile for $E_a = 6$ and 12 and $v = 10^8$ at the instant of time $t = 5$. Here, as well as in the basic sets of other calculations for the 0.6 mm region at the time $t = 0$, the following values were used:

$$\rho = 2, \quad p = 32, \quad U = 4, \quad a = 1$$

For $x \geq 0.6$ it was assumed that $\rho = 1$, $p = 0$, $U = 0$, $a = 1$, while a vacuum was assumed for $x < 0$.

The results of calculations show that for $v = 10^8$ and $E_a = 6$ one obtains a sufficiently close agreement with the analytical solution (heavy line in Fig. 1) corresponding to an instantaneous release of energy. The wide range of v values (from 10^8 to 10^{10}) has no significant effect on the distribution of other properties.

3. In order to determine the structure of the chemical zone, the following changes were made in the computation procedure. In addition to the quadratic numerical Neumann–Richtmayer viscosity, a linear viscosity

$$\varepsilon = \alpha C^2 \frac{d\rho}{dt} \tau \tag{3.1}$$

where C is the velocity of sound and α is a numerical coefficient was also used for calculating the gas dynamics.

The introduction of this linear viscosity made it possible to evade the monotonicity in the property profiles behind the wave front. Coefficient α was chosen so as to render the error thus incurred less than 1-3%.

The other change in the described computation procedure was that the kinetics was figured only behind the shock wave front, the position of this front having been determined on the basis of the highest viscosity number. With such a delayed inclusion of the kinetics in the analysis, it became possible to separate the combustion zone from the zone of pressure buildup at the wave front.

Ahead of the detonation wave one assumed $E = 0$, $U = 0$, $\rho = 1$. The heat of explosion was assumed equal to 4. Under such conditions, and according to the hydrodynamic theory, the parameters of a normal detonation wave are $p^* = 32$ and $\rho^* = 2$, while in the Jouget mode they are $p_J = 16$ and $\rho_J = 4/3$. The characteristics shown here are close to the detonation characteristics of powerful explosive materials such as hexogen and TEN. This encourages one to hope that the obtained results and conclusions concerning the chemical zone profile and the detonation buildup may be applicable to certain compact explosive mixtures.

The parameters in (2.1) were fixed at $E_a = 6$ and $v = 40$. This choice of values was based on the condition of approximate agreement between the calculated and the tested characteristic time of a chemical reaction.

With a simplified expression for the adiabatics of an explosive material one may expect to determine correctly the rate of chemical reactions within a narrow interval of pressures generated by the shock wave. For this reason, the amplitude of the initiating pulse was set equal to the amplitude of the peak in the chemical zone after steady-state had been reached.

Strictly speaking, with the kinetic laws as stipulated in (2.1), the steady mode with a chemical zone of constant width cannot exist at finite distances, since completion of a reaction requires infinite time. It is evident here that, when the explosive material is subjected to a compression wave whose amplitude approaches its limiting value according to the hydrodynamic theory, then the zone of energy release will remain approximately constant. It is essential that a plane in which the Jouget condition $D = U + C$ is satisfied be accepted as the boundary of the chemical zone. The finite width is, moreover, a result of an incomplete energy release. In actual calculations, indeed, this plane – henceforth called the Jouget plane – was determined from the condition $U + C = 8$. Therefore, at every computation point one determined the quantity $\Delta = 8 - (U + C)$. Two points were found (where the "diffluence" is minimal and of opposite signs); the pressure and other properties at the Jouget point were determined by interpolation from the diffluence at these points

$$B_J = \frac{|\Delta_+| B_- + |\Delta_-| B_+}{|\Delta_+| + |\Delta_-|} \tag{3.2}$$

In Fig. 2a is shown the (u, x) profile in a planar detonation wave at the instants of time t = 0.5, 1.0, 1.5, and 2.0.

On this diagram have also been plotted the amplitudes of the initiating pulse and the Jouget modes are identified on it.

Corresponding qualitative trends in the detonation buildup based on the hydrodynamic theory are shown in Fig. 2b. The distribution of the parameters is not fixed within the region between the shock wave front and the Jouget plane, but even then it varies with time much less than in the following rarefaction wave behind the Jouget plane.

In the calculated p(x) curves one observes at the shock wave front a somewhat higher pressure (5–8%) than the maximum according to the hydrodynamic theory. This is a consequence of treating the flow of a substance and the release of chemical energy separately in the computation, but this discrepancy will diminish linearly as the computation step is narrowed.

An analysis of pressure variation at a Jouget point as a function of the distance traveled by the detonation wave has shown that, regardless of the ±40% variation in the initiating pulse amplitude, the pressure at a Jouget point does not differ by more than 1% from the pressure in the steady mode as soon as the detona-

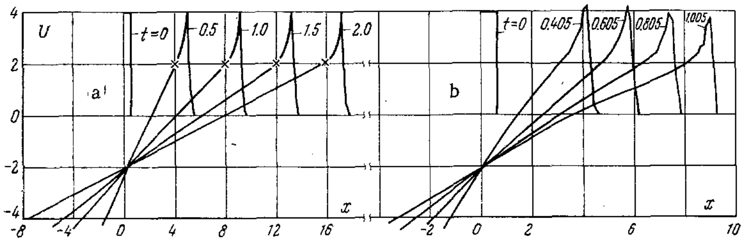

Fig. 2

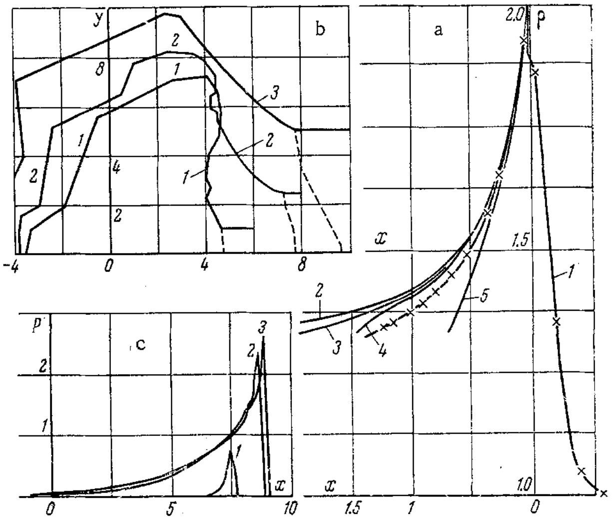

Fig. 3

tion wave has traveled the distance equal to 10 times the characteristic dimension of the chemical zone. In earlier stages the maximum discrepancy amounts to $\Delta p/p_J = 10$ and 3 at times t = 0.2 and 0.4, respectively.

Moreover, a significant widening of the chemical zone at increasing distances was observed within the range of distances for which calculations were made. As the wave continued to propagate, the width of the chemical zone increased from 0.6 (t = 0) to 0.9 (t = 0.5), 1.1 (t = 1.0), and 1.3 (t = 2.0). This widening of the chemical zone causes the pressure to increase at any point of the traveling detonation wave at a fixed distance from the wave front.

A comparison is made in Fig. 3a between the density profile within the chemical zone of a detonation wave which has traveled the distance about 12 mm (curve 1) and the profiles in the steady mode corresponding to various stages of the combustion process: curves 2, 3, 4, and 5 correspond to 0.01%, 0.1%, 0.3%, and 10% unburned substance content at a Jouget point.

The steady-state distribution of parameters in the chemical zone was determined by the method of [2].

We show here the concentrations of explosive material during combustion at Jouget points at various instants of time

$t = 0.2$	0.4	0.6	0.8	1.0	1.2	1.4	1.6
$n = 1.498$	0.892	0.562	0.472	0.438	0.385	0.323	0.323

In the wave which has traveled the distance equal to 10 times the characteristic dimension of the chemical zone, as is evident from Fig. 3a, the density distribution is sufficiently close to that in the steady state.

4. In calculating the detonation of cylindrical charges (diameter 2, 5, and 10 mm) the charge was initiated at the end surface by a pulse of the same amplitude as for the one-dimensional calculations (Fig. 2a).

The exhaust of explosion products into vacuum proceeded from the end surface as well as from the lateral surface of the charge. As had been pointed out earlier, the width of the chemical zone within the range of calculations was about 1 mm. The shape of the boundary and the position of the shock wave front are indicated in Fig. 3b for the instant of time t = 1. For a cylindrical charge 10 mm in diameter one observes a termination into the self-sustaining mode. In Fig. 2b is shown the (U, x) profile along the charge axis during the first few instants of time.

Until t = 0.5 there occurs a lateral discharge toward the axis. Although after that instant of time the axial distributions of the parameters retain their original form, their rate of change, as was to be expected, is higher than in the one-dimensional case. On the other hand, the peak values of the parameters are lower.

One may conclude, on the basis of supplementary calculations for instant of time t = 3 (these calculations were performed with fewer points), that the process terminates into the self-sustaining mode.

In Fig. 3c are shown the pressure profiles for various charge layers at the instant of time t = 1 (curve 1 for the surface layer, curve 3 for the cylinder axis). A pressure drop from the axis to the periphery is clearly evident here.

Detonation calculations for a cylindrical charge 2 mm in diameter (curve 1 in Fig. 3b) have shown that this diameter is subcritical under the given kinetic conditions; owing to the lateral exhaust, the detonation fades out while the explosive material ceases to burn, and after some instant of time the shock wave is propagated along the charge.

The 5-mm diameter (curve 2 in Fig. 3b) turned out to be close to critical. In this case the velocity of the detonation wave is less than normal: One observes a standoff between the combustion front and the shock front. The results obtained in calculating critical diameters of cylindrical charges agree with the Khariton criterion.

5. The results of calculations presented here show that the buildup of the detonation can be analyzed thoroughly enough by an elaborate program. Even with a highly approximated description of the explosive material properties and of the fission kinetics one will obtain numerical detonation characteristics and one will detect certain regularities which are quite realistic.

One may hope, therefore, that a choice of more precise equations of state and an assumption of more realistic and experimentally verified kinetic relations will aid in the analysis concerned with various aspects of the detonation phenomenon and will yield reliable quantitative data.

It follows from the calculations for a one-dimensional flow that already at short distances traveled by the wave one observes a qualitative correlation with the hydrodynamic theory, while at larger distances (narrow width of the chemical zone) the quantitative agreement is fair.

The two-dimensional flow behind a detonation wave front from charges of finite dimensions is more complex. In this case it is not improbable that calculations may reveal features which hardly could be predicted on the basis of simplified models.

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