NUMERICAL CALCULATION OF PARAMETERS OF TWO-LAYER DETONATION

A. M. Mardashev

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In elongated charges of a high explosive (HE) with lengthwise channels, a super-high-speed self-sustaining process can arise if a sufficiently intensive shock wave is propagated in the matter filling the channel. To strengthen this effect the charge can be lined and insulated by a shell from the external medium. A channel wave in such a system acts as an induction source and is self-sustaining at the expense of the compression of the central flow behind the front by expanding reaction products. The general pattern as well as the principal basis for this process – called a "two-layer detonation" – were given in [1]. Confirmation of an actual existence of a two-layer detonation can be found in [2-4]. For the gasdynamic interaction of two layers to be more concrete the detonation of a cylindrical system with a tubular charge of a sensitive HE was considered in [5]. A procedure was proposed for numerical calculation of the parameters of a two-layer detonation in the case of the process velocity exceeding considerably the detonation velocity of the HE. An analytic calculation [6] based on the assumption of uniform distribution of the parameters in the critical section may find very wide application.

1. Outline of the Process and Formulation of the Problem. To investigate a two-layer detonation in cylindrical systems an idealized axially symmetric process is considered as shown schematically in Fig. 1. The scheme refers to systems with sensitive charges. In a laboratory reference system the process is stationary, that is, it does not vary with time. Two layers of matter proceed from the left with velocity U > D where D is the usual velocity of the detonation of the HE. The shock front 0 gives rise to instantaneous initiation of the HE, resulting in the detonation front 1 being formed at some angle determined by the ratio D/U. In the domain W the central flow receives additional compression, which is essential for sustaining the main wave. The domain of the detonation products (DP) Ω has clear-cut boundaries 2 and 3 with the central flow and the shell.

In compliance with the described model it can be assumed that in the domains W and Ω two-dimensional stationary equations of gasdynamics are valid under quite obvious boundary conditions: on 0, the Hugoniot relations; on 1, the state at the detonation front; and on 2 and 3, the conditions on the contact surfaces and the momentum equation characterizing the motion of the shell. In the cylindrical coordinate system r-z corresponding to the symmetry axis and the front 0 of the head wave, the respective equations for a polytropic gas (\varkappa) in the domain Ω are given by

 $\begin{aligned} u\partial\rho/\partial r + \omega\partial\rho/\partial z + \rho(\partial u/\partial r + \partial\omega/\partial z + u/r) &= 0. \\ u\partial u/\partial r + \omega\partial u/\partial z + (1/\rho)\partial p/\partial r &= 0, \\ u\partial\omega/\partial r + \omega\partial\omega/\partial z + (1/\rho)\partial p/\partial z &= 0, \\ u\partial\rho/\partial r + \omega\partial\rho/\partial z + \varkappa p(\partial u/\partial r + \partial\omega/\partial z + u/r) &= 0, \end{aligned}$ (1.1)

where u and ω are radial and axial velocity components, the remaining notation being generally acceptable. The independent variable z is replaced in the system (1.1) by t by means of the formula

$$z = Ut.$$

If one now omits in the equations such terms as $\partial (\omega/U-1)F/\partial t$, one obtains a one-dimensional system of gasdynamic equations and a single equation for ω , which is ignored from now on:

$$\frac{\partial \rho}{\partial t} + u \partial \rho / \partial r + \rho (\partial u / \partial r + u / r) = 0,$$

$$\frac{\partial u}{\partial t} + u \partial u / \partial r + (1/\rho) \partial \rho / \partial r = 0,$$

$$\frac{\partial \rho}{\partial t} + u \partial \rho / \partial r + \kappa \rho (\partial u / \partial r + u / r) = 0.$$
(1.2)

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The system (1.2) is at least applicable to processes such that $U \gg D$. If this condition is considered as satisfied, we formulate the relevant boundary conditions.

The parameters on the 1 boundary are specified by the state at the strong detonation wave, which is given by the values of \varkappa , D and of the HE density ρ_1 :

$$\rho_D = [(\varkappa + 1)/\varkappa]\rho_1, \ p_D = \rho_1 D^2/(\varkappa + 1), \ u_D = D/(\varkappa + 1).$$
(1.3)

To obtain a boundary condition on the boundary 2 one assumes the central flow to be also a polytropic gas (γ) , and bearing in mind that for U \gg D the cross velocities are negligibly small compared with the lengthwise ones, the flow is now described by the simple equations of a quasi-one-dimensional model:

$$\omega^2/2 + [\gamma/(\gamma - 1)]p/\rho = \text{const}, \qquad (1.4)$$

$$p/\rho^{\gamma} = \text{const}, \ \rho\omega(f/r_0)^2 = \text{const},$$

where f is the current radius of the central flow whose initial radius is denoted by r_0 . The radius f is regarded either as a function of t or of z depending on our requirements. The constants on the right of (1.4) are determined by the parameters on the strong shock wave 0:

$$\rho_y = [(\gamma + 1)/(\gamma - 1)]\rho_0, \ p_y = [2/(\gamma + 1)]\rho_0 U^2, \ \omega_y = [(\gamma - 1)/(\gamma + 1)]U,$$

where ρ_0 is the density of the unperturbed flow. By solving the system (1.4) for p and f one finds the sought boundary condition:

$$[4\gamma/(\gamma-1)^2](p/p_u)^{(\gamma+1)/\gamma} [(\gamma+1)/(\gamma-1)]^2(p/p_u)^{2/\gamma} + (r_0/f)^4 = 0.$$
(1.5)

On the boundary 3 one uses the momentum equation for a shell in motion, which can be obtained from the equations of the incompressible and ideally plastic medium:

$$mdu(\varphi)/dt = p(\varphi) - Y\delta/\varphi, \qquad (1.6)$$

where m is the shell mass per unit area of the bounding surface; Y is the dynamic yield limit; δ is the variable shell thickness; and φ is the current radius of the inner boundary of the shell.

To these boundary conditions on the surfaces 2 and 3 one adjoins the equations of no leaking:

$$df/dt = u(f), \ d\varphi/dt = u(\varphi). \tag{1.7}$$

Thus, in the one-dimensional approximation and with known U the problem (1.2), (1.3), (1.5)-(1.7) is formulated to determine the unknown functions ρ , p, u in the transformed Ω domain and also to find its boundaries f and φ ; having changed over to the previous variable z, their solution determines the parameters of the twolayer detonation.

2. Computation Procedure. In the original data the free parameter U is varied and the problems thus arising are solved numerically. The solution of each successive problem should each time be nearer to the sought one, which differs in that in the central flow the sound velocity is reached with regard to the channel wave. This condition is necessary for a stationary subsonic flow past the discontinuity. It can be shown starting with Eqs. (1.4) that the sound velocity in the quasi-one-dimensional flow under consideration is only attained in a specified section of highest compression, which is called critical; its radius r_* is calculated by using, first of all, the formula

$$r_{\star}/r_{0} = [(\gamma - 1)/(\gamma + 1)]^{1/4} [2\gamma/(\gamma + 1)]^{1/(2(\gamma - 1))}.$$
(2.1)

The nearness to the sought solution is judged by the difference $r_m - r_*$, where r_m is the radius of maximal compression of the central flow in the numerical solution. The assumption is made when adopting a value of the free parameter that the solutions depend continuously on the initial data; the latter, and also the taking into account of some physical considerations, enable one to estimate the value of the varied parameter for the next step of the calculation.

TABLE 1

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No. of variants	ρ₀, g/cm ^s	ρ1, g/cm ³	ρ2, g/cm ³	r ₁ /r ₉	δο	a, km/sec	λ	Y , kbar	z_m'ro	U, km/sec
1 2 3 4 5 6 7	0,070 0,071 0,071 0,071 0,071 0,071 0,070	1,72 1,68 1,68 1,68 1,68 1,72	7,8 2,78 2,78 7,85 7,85	1,4 2 3 2 3 4,4	0,5 1 1 1 1 1	3,8 5,32 5,32 4,56 4,56	1,58 1,33 1,33 1,49 1,49 1,49	9,8 3,9 3,9 9,8 9,8 9,8	2,8 5,6 10,0 6,1 11,2 4,9	10,1 10,9 11,4 11,5 11,9 12,9



One should now note some essential features of the numerical algorithm used to solve the ensuing problems.

There are two singular points in the domain Ω : the initiation point at which the computation starts and the reflection point of the detonation wave from the shell. Since the solutions of the problems in the break-ups of planar or of curved breaks in a sufficiently small time interval are as close as desired, the unknown functions in the neighborhood of these points are determined by the solutions of the following one-dimensional problems: 1) the motion of the detonation products arising between the front of the strong detonation wave started on the surface of a semiinfinite charge and the free surface with pressure specified on it; 2) the reflection of the strong detonation wave from the two-dimensional deformed obstacle.

The computational difficulties due to the moving piecewise-smooth boundary can be overcome by using the procedure described in [7], although in a pure form it is not appropriate for finding a discontinuous solution. Therefore, when the detonation wave is reflected, smoothing has to be carried out in parallel [8].

The numerical algorithm keeps the computational error also under control. At some instants t, by using discrete values of the parameters of the numerical solution, the errors are determined in the integral laws of conservation of mass and energy, which are then related to the mass and chemical energy of the charge per unit length. The relative errors thus obtained are then printed out. All the main points of the numerical algorithm are described in more detail in [5].

3. Computational Results. The procedure we have just described was applied to compute approximately the parameters of a two-layer detonation in a real situation. The computations were carried out to determine whether it is possible to obtain higher velocities at the loading of liquid hydrogen by charges of pressed Hexogen. To this end, 11 variants of the initial data were adopted corresponding to cylindrical systems with different charge volumes contained in Duralumin, in steel, or in an absolutely rigid shell. For the liquid hydrogen one has $\gamma = 1.4$ and 1.67. Two parameters relevant to the HE remain unchanged: $\varkappa = 3$ and D = 8.5 km/sec. The velocity U and other parameters of the two-layer detonation were determined by the parameters of that problem for which $r_m - r_* \le 0.02r_0$. In solving successive problems with U reduced by 0.1 km/sec, the current radius f assumed also the value r_* , but for df/dt < 0.

The main results obtained for $\gamma = 1.4$ are shown in Table 1, where ρ_2 is the density of the shell material; r_1 is the outer charge radius; δ_0 is the initial shell thickness; *a* and λ are empirical constants in the expression for the linear dependence of the shock-wave velocity on the mass velocity at the front for the material of the shell; and z_m is the distance between the front of the channel wave and the maximal compression section of the central field (the last parameter characterizes the error of the model due to the mass exchange between the DP and the mass of the central flow being neglected). One can see that due to the adopted initial data the scattering of the velocities is rather small (within 10.1-15.8 km/sec). The effect of r_1 , ρ_2 on z_m and U is different. For example, if the thickness of the HE grows from r_0 to $2r_0$, the distance z_m is approximately double U, increasing at the same time by less than 0.5 km/sec. The greatest increment of U occurs when the shell remains stationary; this can be verified by comparing the first and the last two variants.

In accordance with the assumptions of the employed model, the variants with the highest U and the lowest z_m yield the most accurate estimates of real parameters of a two-layer detonation. Using this approach one can find some variants with close U and z_m . In particular, the variant $z_m/r_0=5.6$, U=10.9 km/sec corresponds to the conditions in an actual experiment [4]. The mean velocity of the process under consideration is almost identical with the computed one. It follows from the calculations as well as from the formulas of [6] that there are limited possibilities of obtaining very high velocities for the systems under consideration: the limiting velocity calculated for $r_1 \rightarrow \infty$ by using the formulas of [6] is 22.82 km/sec.

In Fig. 2 the DP limits are shown in the variables r/r_0 and z/r_0 for the variants with a moving shell and $\gamma = 1.4$; the dashed line corresponds to the value of $r/r_0 = 0.7747$ obtained for the specified γ using the expression for r_*/r_0 of (2.1) (the numerals are the variant ordinals). The inclination of the boundary of the central flow to the axis of symmetry df/dz (dimensionless quantity) may assume negative or positive (but always low) values. It can be shown that for all variants the estimate

$$|df/dz| \leqslant 0.21 \tag{3.1}$$

is valid. The corresponding estimate for the inclination of the DP boundaries is not worse than (3.1), which justifies the use on the one-dimensional boundary conditions (1.5) and (1.6) of the DP lateral boundaries.

The computation results for $\gamma = 1.67$ do not differ qualitatively from those of $\gamma = 1.4$ and are thus omitted.

The discussed results were obtained using a grid with 20 computation nodes of the space variable. As regards the mass and energy equilibrium, their deviations did not exceed 4.5% for variants with shells remaining constant, r_m and z_m being determined with a satisfactory accuracy. Thus, the checking of the second variant on a grid twice reduced showed that the relative error did not exceed 2%. With the value of U obtained from the original grid the change in r_m was only in the fourth decimal place and z_m was reduced by 0.077 r_0 . For this case the distributions of p/pp in some DP cross sections against the dimensionless variable $\mu = (r-f)/(\varphi - f)$, $f \le r \le \varphi$ are shown in Fig. 3; one can see now that for $z/r_0=2.6$ the wave reflected from the shell is weak, but the irregularity of pressure distribution is maintained up to the critical section ($z/r_0=5.6$). The irregularity of pressure distribution in the critical section is a characteristic feature of all variants and it appears strongly in the last two variants with shells not in motion. In Fig. 4, dimensionless pressure profiles in the critical section are shown for them, where the numerals over the curves are the ordinal numbers of the appropriate variant.

4. Justification of One-Dimensional Approximation. The proposed approach for evaluating the parameters of a two-layer detonation is based on the numerical solution of Eqs. (1.2). To justify the use of an approximation an estimate is given in the calculation range of the quantity $(\omega/U-1)$.

At the detonation front the axial component of velocity is known:

$$\omega_n = U - [1/(\kappa + 1)]D^2/U. \tag{4.1}$$

With the extension of the DP the mean velocity increases monotonically in the critical section up to the value ω_* . For variants with immobile shells ω_* is evaluated directly using the analytic formulas of [6], since they remain valid for any ratios of U and D. They also remain valid with some slight corrections for variants with moving shells. One must know in addition the momentum G₁ transmitted to the shell in the axial direction per unit of time as well as φ_1 , which is the value of φ in the critical section. If the central matter does not react chemically and the Mach numbers M of the channel wave are sufficiently high (quantities of the order of $1/M^2$ can be ignored) simple equations are obtained for the velocities ω_* and U:

$$\omega_*/U = \alpha - \beta/(\kappa + 1),$$

$$(D/U)^2 = 1 + \kappa^2(\alpha^2 - 1) - (\beta - \alpha)^2,$$

$$= 1 + BZG(1 + G_2/G_2), \quad \beta = RPS(\kappa + 1),$$

(4.2)

TABLE 2

Vari- ant No.	R	z	Q_1/Q_0	φ_1/r_0	s	α	β	ω_*/U	U, km/ sec
1 2 3 4 5 6 7	0,041 0,042 0,042 0,042 0,042 0,042 0,041 0,042	$\begin{array}{c} 1,042\\ 0,333\\ 0,125\\ 0,333\\ 0,125\\ 1,042\\ 0,333\end{array}$	1,54 4,79 12,0 3,96 10,12 0 0	1,6 2,49 3,57 2,58 3,89 1,4 2	$\begin{array}{c} 2,042\\ 1,867\\ 1,518\\ 2,019\\ 1,816\\ 1,417\\ 1,133\end{array}$	$\begin{array}{c} 1,032\\ 1,024\\ 1,020\\ 1,021\\ 1,017\\ 1,013\\ 1,004\\ \end{array}$	0,162 0,152 0,124 0,164 0,148 0,113 0,092	0,99 0,99 0,99 0,98 0,98 0,98 0,98	9,3 10,3 11,3 10,5 11,4 13,0 17,3

where $R = \rho_0 / \rho_1$; $Z = r_0^2 / (r_1^2 - r_0^2)$; $S = (\varphi_1^2 - r_*^2) / (r_1^2 - r_0^2)$; G_0 is the momentum transmitted to the central flow in the axial direction in a unit of time; and G and P are functions of γ , namely,

$$G = 1 - \frac{\sqrt{\gamma^2 - 1}}{\gamma}, \quad P = \frac{2}{\gamma + 1} \left(\frac{\gamma + 1}{2\gamma}\right)^{\gamma/(\gamma - 1)}.$$

For the ratios D/U and ω_*/U their definition domain is given by

$$\boldsymbol{\alpha} \ge \mathbf{1}, \ \boldsymbol{\beta} \ge 0, \ \boldsymbol{\alpha} \ge \boldsymbol{\beta}. \tag{4.3}$$

The first two constraints of (4.3) result from the physical meaning of the initial data which define α and β , the third is the condition for the supersonic flow of the DP to be present in the critical section.

In numerical experiments with liquid hydrogen one had to bear in mind that the initial pressure was of the order of 1 atm. The obtained values of the velocities of the channel waves are $M \ge 10$ which enables one to employ the formulas (4.2).

Let the above-calculated 11 variants Q_0 and Q_1 be the numerical values of the work accomplished by the DP on a unit length of inner or outer surface. Then the relations

$$G_0 = \int_{r_0}^{r_s} p 2\pi f df \simeq Q_0, \quad G_1 \simeq Q_1$$

are valid, and this enables one to replace G_1/G_0 in the expressions for α by Q_1/Q_0 . If for φ_1 one uses the numerical values of φ for z_m , then α and β and hence, ω_* and U, can be calculated.

The initial data as well as the computation results using the formulas (4.2) for $\gamma = 1.4$ are given in Table 2; it can be seen that all the α and β pairs satisfy the inequalities (4.3), and that the ratios ω_*/U are close to unity. Using (4.1) it can be established that for all variants one has

$$-0.02 \geqslant \omega/U - 1 \geqslant -0.2.$$

Under such constraint the comparison of the values of U from Table 1 and Table 2 obtained in a different manner shows that the terms of the form $\partial (\omega/U-1)F/\partial t$ have no marked effect on the velocity of the two-layer detonation. It is obvious that the discrepancy in the last variant is due to the lack of parameter uniformity in the critical section.

In the general case, it follows from (4.1) and (4.2) that

$$\max_{D/U=\text{const}}\left(\frac{\omega_{*}}{U}-1\right)=\sqrt{1+\frac{1}{\varkappa^{2}-1}\left(\frac{D}{U}\right)^{2}}-1\geqslant\frac{\omega}{U}-1\geqslant-\frac{1}{\varkappa+1}\left(\frac{D}{U}\right)^{2}.$$

These relations provide a basis for the use of one-dimensional approximation not only for $U \gg D$, but also if U is comparable with D.

It should be mentioned that for the boundary conditions of the problems under consideration to be determined with regard to the starting parameters ρ_0 and U one only needs to know the product $\rho_0 U^2$. The latter enables one to extend the numerical results to the processes in which ρ_0 and U vary over wide ranges but such that the product $\rho_0 U^2$ remains constant.

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GENERATION OF A PLANE RELAXATION WAVE IN AN AEROCOLLOIDAL SUSPENSION OF SOLID PARTICLES

A. D. Gol'tsiker, S. V. Tarakanov, O. M. Todes, and S. A. Chivilikhin UDC 532.593;541.182.3

The analysis of propagation of a stationary shock wave in an aerocolloidal suspension [1-4] has shown that behind the shock front is a rather broad relaxation zone, in which the suspended particles are gradually accelerated by the gas flow. In that zone the particles are heated up to the temperature of the gas, heat is released due to the work of friction forces, and various phase transitions are possible, for example, melting and evaporation of the colloidal particles. It is exceedingly difficult to obtain an analytic solution of the system of differential equations describing the gas and particles; as a rule, a computer is recruited as an aid to finding solutions for various special cases.

Even more insurmountable are the mathematical difficulties associated with investigation of the transient part of shock generation in an aerocolloid, as in the case, for example, when a shock wave traveling through a pure gas impinges on a domain filled with an aerocolloid.

For a small volume concentration of particles the leading edge of the shock wave enters the aerocolloid virtually unchanged. Immediately, however, two contact surfaces are formed: 1) the boundary of the moving cloud of particles; 2) the boundary (interface) between the original (before arrival of the shock) dusty gas and the clean gas.* The particles set in motion generate disturbances in the surrounding medium in the form of rarefaction and compression waves. Inasmuch as the leading edge of the shock waves moves relative to the trailing gas at less than the velocity of sound, the disturbances overtake the shock front and begin to deform it. Finally a reflected shock is formed and propagates in the opposite direction.

*The second boundary is logically called the gas contact surface. Its trajectory is clearly the trajectory of the gas mass present at the initial instant at the nonmoving interface between the gas and aerocolloid.

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