- 10. M. P. Slavinskii, Physicochemical Properties [in Russian], Nauka, Moscow (1960).
- 11. R. McQueen and S. Marsh, J. Appl. Phys., <u>31</u>, No. 7, 1253 (1960).
- 12. S. B. Kormer and V. D. Urlin, Dokl. Akad. Nauk SSSR, 131, No. 3, 542 (1960).
- 13. I. I. Frantsevich and F. F. Voronov, Elastic Constants and Elastic Moduli of Metals and Nonmetals [in Russian], Nauka, Moscow (1982).
- 14. V. A. Zhdanov and A. V. Zhukov, Prikl. Mekh. Tekh. Fiz., No. 5, 139 (1978).
- S. N. Ishutkin, G. E. Kuz'min, and V. V. Pai, Fiz. Goreniya Vzryva, <u>22</u>, No. 5, 96 (1986).
 J. Taylor, J. Appl. Phys., 34, No. 9, 2727 (1963).
- 17. L. V. Al'tshuler, S. B. Kormer, A. A. Bakanova, et al., Zh. Éksp. Teor. Fiz., <u>38</u>, No. 3, 790 (1960).
- 18. K. Gschneider, Solid State Phys., <u>16</u>, 275 (1964).

EQUATION OF STATE OF DETONATION PRODUCTS OF COMPACT EXPLOSIVES

V. F. Kuropatenko

The behavior of detonation products (DP) of compact explosives is described satisfactorily in a number of cases by the equation of state [1-3]

$$p = f(\rho) T + \varphi(\rho), \tag{1}$$

which takes account of the molecule interaction in a broad range of variation of the temperature T and density ρ . In a number of cases the functions $f(\rho)$ and $\phi(\rho)$ are selected in simplest form. Thus a simple dependence of the pressure p on the density

$$p = A \rho^n \tag{2}$$

UDC 622:215

is proposed in [2] to describe the DP properties in the neighborhood of the Jouget point. The equation of state

$$p = B_0 T + A_0^n \tag{3}$$

with three constants is examined in [1]. The equations of state (2) and (3) have a limited range of applicability. If the numerical values of A, n, B are chosen such that the error would be least in the neighborhood of the Jouget point, then it will grow noticeably with distance from it along the isentrope. The flinging properties of explosives are described better and the parameters of the normal detonation wave (DW) worse for another choice of constants. In order to increase the accuracy of describing DP behavior in the neighborhood of the Jouget point under isentropic expansion and moderate compressions, a number of equations of state [4-6] of the type (1) was created with different functions $f(\rho)$ and $\phi(\rho)$ containing around 10 constants. The rise in their accuracy is achieved by noticeable complication. It is characteristic for the mentioned equations of state of the DP that the numerical values of the major part of the parameters therein are determined individually for each explosive.

Let us consider one of the methods for finding the functions $\gamma(\rho)$ and $\phi(\rho)$ for (1)

$$p = (\gamma(\rho) - 1)\rho E + \varphi(\rho). \tag{4}$$

A physical experiment permits determination of the dependence of the velocity D of the normal detonation wave, the mass flow rate u behind the wave front, and the calorific value Q of the explosive on the initial density ρ_0 ahead of the detonation wave front. We will use these dependences to set up the form of the functions $\gamma(\rho)$ and $\phi(\rho)$ and to determine the numerical values of the parameters in them.

The conservation laws on a strong discontinuity with instantaneous liberation of internal energy Q have the form

Chelyabinsk. Translated from Fizika Goreniya i Vzryva, Vol. 25, No. 6, pp. 112-117, November-December, 1989. Original article submitted April 5, 1988.

$$\rho(D-u) = \rho_0(D-u_0), \quad p-p_0 = \rho_0(D-u_0) (u-u_0),$$

$$E-E_0 = 0.5 (u-u_0)^2 + p_0(u-u_0) / \rho_0(D-u_0) + Q,$$

$$D = u + c, \quad c^2 = \left(\frac{\partial P}{\partial \rho}\right)_8.$$
(5)

For a given equation of state (4) the system (4) and (5) determines the line of the Jouget points on which all the thermodynamic quantities and velocities depend on ρ_0 . Let us introduce the concept of a crystalline or greatest possible explosive density ρ_{0K} under normal conditions and a normal detonation wave velocity D_K in an explosive with this density. Let us use ρ_{0K} and D_K to go over to dimensionless variables

$$\Delta = \rho_0 / \rho_{0\mathrm{K}}, \quad \delta = \rho / \rho_{0\mathrm{K}}, \quad W = D / D_{\mathrm{K}},$$

$$M = u / D_{\mathrm{K}}, \quad Z = c / D_{\mathrm{K}}, \quad \Pi = p / \rho_{0\mathrm{K}} D_{\mathrm{K}}^2,$$

$$\Phi = \varphi / \rho_{0\mathrm{K}} D_{\mathrm{K}}^2, \quad J = E / D_{\mathrm{K}}^2, \quad K = Q / D_{\mathrm{K}}^2.$$
(6)

For simplicity we shall consider $u_0 = 0$, $p_0 = 0$, $E_0 = 0$ in (5). After having gone over to the dimensionless variables (6), the equations (5) become

$$\delta = W\Delta/(W - M), \quad \Pi = WM\Delta,$$

$$J = 0.5 M^2 + K, \quad W = M + Z, \quad Z = \left(\frac{\partial \Pi}{\partial \delta}\right)_S.$$
(7)

Let us write (4) in dimensionless variables

$$\Pi = (\gamma - 1)\delta J + \Phi. \tag{8}$$

The system of six equations (7) and (8) contains nine functions of Δ : II, δ , J, W, M, K, Z, γ , ϕ . The system becomes definite if any three of the nine mentioned functions of Δ are given, i.e., are defined without utilization of (7) and (8).

Let us introduce the index of adiabaticity N

$$N = \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_{S}.$$
(9)

Going over to dimensionless quantities and using (5) and (7), we obtain

$$N = Z^2 \delta / \Pi. \tag{10}$$

Let us eliminate Z and M in (7) and (10)

$$\delta = \Delta (N+1)/N, \quad \Pi = W^2 \Delta/(N+1),$$

$$J = \frac{W^2}{2(N+1)^2} + K, \quad \left(\frac{\partial \Pi}{\partial \delta}\right)_S = \left(\frac{WN}{N+1}\right)^2.$$
 (11)

Let us find an expression for the derivative $(\partial \Pi / \partial \delta)_S$. To do this, we use the thermodynamic equation

$$\left(\frac{\partial\Pi}{\partial\delta}\right)_{S} = \left(\frac{\partial\Pi}{\partial\delta}\right)_{J} + \left(\frac{\partial\Pi}{\partial J}\right) \left(\frac{\partial J}{\partial\delta}\right)_{S}.$$
 (12)

It follows from the main thermodynamics equations that along the isentrope

$$\left(\frac{\partial J}{\partial \delta}\right)_{S} = \frac{\Pi}{\delta^{2}}.$$
(13)

Let us substitute expressions for the derivatives

$$\left(\frac{\partial\Pi}{\partial\delta}\right)_{J} = \frac{d\Phi}{d\delta} + (\gamma - 1)J + \delta J \frac{d\gamma}{d\delta}, \qquad (14)$$

$$\left(\frac{\partial \Pi}{\partial J}\right)_{\delta} = (\gamma - 1)\,\delta\tag{15}$$

into (12) and let us eliminate $(\partial J/\partial \delta)_S$ by using (13)

$$\frac{d\Phi}{d\delta} + (\gamma - 1)J + \delta J \frac{d\gamma}{d\delta} + \frac{(\gamma - 1)\Pi}{\delta} - \left(\frac{WN}{N-1}\right)^2 = 0.$$
(16)

Using (8) we eliminate J in (16). We consequently obtain

$$\frac{d\Phi}{d\delta} - \frac{\Phi}{\delta} + \frac{(\gamma - N)\Pi}{\delta} + \frac{(\Pi - \Phi)}{\gamma - 1} \frac{d\gamma}{d\delta} = 0.$$
(17)

All the quantities on the line of Jouget points depend on Δ . Let us replace differentiation with respect to δ by differentiation with respect to Δ in (17). To do this, we first differentiate δ with respect to Δ :

$$\frac{d\delta}{d\Delta} = \frac{N-1}{N} - \frac{\Delta}{N^2} \frac{dN}{d\Delta}.$$
(18)

Multiplying (17) by $d\delta/d\Delta$, we obtain

$$\frac{d\Phi}{d\Delta} + \left(\frac{(\gamma - N)\Pi}{\delta} - \frac{\Phi}{\delta}\right) \left(\frac{N - 1}{N} - \frac{\Delta}{N^2} \frac{dN}{d\Delta}\right) + \frac{\Pi - \Phi}{\gamma - 1} \frac{d\gamma}{d\Delta} = 0.$$
(19)

Using (8) and (11) we express Φ in terms of Π , δ , N and K:

$$\Phi = \Pi - \frac{(\gamma - 1) \Delta (W^2 - 2K (N + 1)^2)}{2N (N + 1)}.$$
(20)

Using (18) we eliminate Φ in (17). To eliminate $d\Phi/d\Delta$ also, we proceed as follows. We substitute the expression for I from (11) into (20) and differentiate the expression obtained with respect to Δ

$$\frac{d\Phi}{d\Delta} = \frac{W^2}{N+1} - \frac{(\gamma-1)\left(W^2 + 2K\left(N+1\right)^2\right)}{2N\left(N+1\right)} + \frac{W\Delta\left(2N-\gamma+1\right)}{N\left(N+1\right)} \frac{dW}{d\Delta} - \frac{(\gamma-1)\left(N+1\right)\Delta}{N} \frac{dK}{d\Delta} + \left(\frac{W^2\Delta\left(\gamma-1-N\right)}{N\left(N+1\right)^2} - \frac{(\gamma-1)K\Delta\left(2N+1\right)}{N^2}\right)\frac{dN}{d\Delta} - \frac{\Delta\left(W^2 + 2K\left(N+1\right)^2\right)}{2N\left(N+1\right)} \frac{d\gamma}{d\Delta}.$$
(21)

Substituting (20) and (21) into (19), we obtain the equation of the Jouget line

$$W\Delta(2N-\gamma+1)\frac{dW}{d\Delta} - (\gamma-1)(N+1)^2\Delta\frac{dK}{d\Delta} + NW^2(\gamma-N) = 0.$$
(22)

that contains three functions of Δ (W(Δ), K(Δ), N(Δ)) that can be measured experimentally. After having determined the functions mentioned, the expression (22) permits finding the dependence

$$\gamma = 1 - \frac{2\Delta NW \frac{dW}{d\Delta} - NW^2 (N-1)}{W\Delta \frac{dW}{d\Delta} + (N+1)^2 \Delta \frac{dK}{d\Delta} - NW^2}.$$
(23)

It follows from (23) that there are certain connections between W, N and K. Since $\gamma \ge 1$ then the numerator and denominator in (23) should vanish simultaneously. For many explosives these W(Δ) are described with satisfactory accuracy by the dependence

$$W = \Delta^{\alpha}, \tag{24}$$

where $\alpha \approx 0.7$. Substituting (24) into (23) and introducing the notation $\omega = \Delta^{1-2\alpha} dK/d\Delta$, we obtain

$$\gamma = 1 + \frac{N(N-1-2\alpha)}{N-\alpha-\omega(N+1)^2}.$$
(25)

Let us introduce another set of additional constraints on the nature of the functions $N(\Delta)$ and $\omega(\Delta)$. Let us demand that $N \Rightarrow \gamma \Rightarrow \gamma_0 = \text{const} \text{ as } \Delta \Rightarrow 0$. For small ρ we consider the equation of state (4) for $\gamma = \gamma_0$. We represent p and E in the form of the hot and cold components

$$p = p_{\rm r}(\rho, T) + p_{\rm x}(\rho), \quad E = E_{\rm r}(\rho, T) + E_{\rm x}(\rho).$$
 (26)

Let us consider that

$$p_{\rm r} = (\gamma_0 - 1)\rho E_{\rm r}, \quad E_{\rm r} = c_{\rm v}T, \quad c_{\rm v} = {\rm const.}$$
 (27)

Using (25) and (27) then (4) is

$$pV = (\gamma_0 - 1)c_v T + f(V),$$
 (28)

where

$$f(V) = V\varphi(V) + (\gamma_0 - 1)E_x(V); \quad V = 1/\rho.$$

Let us consider the DP to be a mixture of gases under conditions of mechanical and thermal equilibrium and subject to the equations of state

$$pV_{i} = (\gamma_{0i} - 1)c_{vi}T + f_{i}(V_{i}).$$
⁽²⁹⁾

Using the additivity of V and E in the mixture

$$V = \sum_{i} \varkappa_{i} V_{i}, \quad E = \sum_{i} \varkappa_{i} E_{i}$$
(30)

 $(\kappa_i \text{ is the mass concentration of the i-th component})$, we write (27)-(29) in the form

$$(\gamma_0 - 1) c_V T + f(V) = \sum_i [(\gamma_{0i} - 1) c_{Vi} \varkappa_i T + \varkappa_i f_i(V_i)], \qquad (31)$$

$$c_V T + E_{\mathbf{x}}(V) = \sum_i \left[\varkappa_i c_{Vi} T + \varkappa_i E_{\mathbf{x}i}(V_i) \right].$$
(32)

For T = 0 a relation follows from (31) and (32) between the cold components of the mixture equation of state and the components

$$f(V) = \sum_{i} \varkappa_{i} f_{i}(V_{i}), \quad E_{\mathbf{x}}(V) = \sum_{i} \varkappa_{i} E_{\mathbf{x}i}(V_{i}).$$
(33)

It follows from (30)-(33) that for any value of T there should be

$$(\gamma_0 - 1) c_V = \sum_i (\gamma_{0i} - 1) \varkappa_i c_{Vi},$$
 (34)

$$c_V = \sum_i \varkappa_i c_{Vi}. \tag{35}$$

Therefore, to determine the γ_0 of the mixture it is necessary to know the κ_i , γ_i and c_{Vi} of each component. Such data are presented in [1, 7, 8] for a number of explosives. According to different theories, the mass concentrations of the DP components are distinct. Consequently, we limit ourselves to consideration of the average concentrations. In such an approach

$$\gamma_0 = 1 + \left(\sum_i (\gamma_{0i} - 1) \varkappa_i c_{Vi} \right) / \left(\sum_i \varkappa_i c_{Vi} \right).$$
(36)



Fig. 1

TABLE 1

Explosive	ρ _{0K} , g/cm	D _K , km/sec	Explosive	р _{ок} , g/cm	D _K , km/sec
Trotyl	1,663	7,15	TEN	1,770	8,35
Tetryl	1,730	7,74	Hexogen	1,820	8,80

For trotyl $\gamma_0 = 1.373$, which is close to the value $\gamma_0 = 1.378$ for hexogene. Since this difference lies within the limits of errors allowed for averaging of κ_i , then we take the single value $\gamma_0 = 1.375$ for trotyl and hexogene that is close to $\gamma_0 = 1.33$ taken in [4] for a number of miscible explosives.

Little data on the calorific values of explosives are contained in the literature. Exactly as results on N(Δ), they have a noticeable spread. Let us use data from [1, 3-9] by representing them in dimensionless form and approximating them by single dimensionless dependences on Δ for different explosives. It follows from (22) and (24) that as $\rho \rightarrow 0$, $\Delta \rightarrow 0$ and N $\rightarrow \gamma \rightarrow \gamma_0$ there should be

$$\omega \to \omega_0 = \frac{\alpha}{\gamma_0^2 - 1}.$$
(37)

Furthermore, from the condition of finiteness of γ , i.e., from the condition of simultaneous disappearance of the numerator and denominator in (25), there follows that there should be

$$\omega = \omega_* = \frac{1}{4(1+\alpha)}$$
 for $N = 1 + 2\alpha$. (38)

Moreover, we demand that ω still satisfy two conditions for Δ = 1:

$$\int_{0}^{1} \Delta^{2\alpha - 1} \omega d\Delta = K_{\rm K}, \quad \omega = 0, \tag{39}$$

where KK is the value of the dimensionless caloric value of the explosive for $\Delta = 1$. The conditions (39) are suggested after an analysis of the experimental data on caloric values of explosives. Conditions (37)-(39) and equation (22) substantially constrain the class of functions that can be used to approximate experimental data on K(Δ) and N(Δ).

Because of its awkwardness we omit the procedure for the numerical solution of (22) with conservation of the constraints on $\omega(\Delta)$ and $\gamma(\Delta)$ listed above and with simultaneous optimization of the approximations of the experimental data on the behavior of N(Δ) and K(Δ). We approximate the tabulated dependences obtained, in turn, by the functions

$$\gamma = \begin{cases} \gamma_{\infty} & \text{for } x > 1, \\ \gamma_0 + (\gamma_{\infty} - \gamma_0) x (3 - 3x + x^2) & \text{for } x \leq 1, \end{cases}$$
(40)

$$\varphi = \begin{cases} \rho_{0R} D_{R}^{2} A \left(x-1\right)^{m} & \text{for } x > 1; \\ 0 & \text{for } x \leq 1, \end{cases}$$

$$\tag{41}$$

where x = δ/δ_{*} ; A = 0.0139; γ_0 = 1.375; γ_m = 1.667; δ_{*} = 0.35; m = 2.284.

For a final construction of the DP equation of state for a specific compact explosive the parameters ρ_{0K} and D_K must be determined (they are presented in the table for certain explosives). For miscible explosives the values of ρ_{0K} and D_K are expressed by using the simple equations

$$\rho_{\mathrm{er}} = 1 \left/ \left(\sum_{i} \varkappa_{i} / \rho_{\mathrm{0K}i} \right), \quad D_{\mathrm{K}}^{2} = \sum_{i} \varkappa_{i} D_{\mathrm{K}i}^{2}.$$

A comparison of the functions $W(\Delta)$ (a), $N(\Delta)$ (b) and $K(\Delta)$ (c) (lines) with experimental data from [1, 3-9] is presented in the figure: 1) trotyl; 2) hexogen; 3) TEN; 4) tetryl.

LITERATURE CITED

- F. A. Baum, K. P. Stanyukovich, and B. I. Shekhter, Physics of Explosion [in Russian] Fizmatgiz, Moscow (1959).
- 2. L. D. Landau and K. P. Stanyukovich, Dokl. Akad. Nauk SSSR, 46, 399 (1945).

- 3. K. Johannson and P. Person, Explosive Detonations [Russian translation], Mir, Moscow (1973).
- 4. M. V. Zhernokletov, V. N. Zubarev, and G. S. Telegin, Prikl. Mekh. Tekh. Fiz., No. 4 (1969).
- 5. V. N. Zubarev, Prikl. Mekh. Tekh. Fiz., No. 2 (1965).
- 6. N. M. Kuznetsov and K. K. Shvedov, Fiz. Goreniya Vzryva, <u>1</u>, No. 4, 85 (1965).
- 7. A. N. Dremin, S. D. Savrov, V. S. Trofimov, et al., Detonation Waves and Condensed Media [in Russian], Nauka, Moscow (1970).
- B. Ya. Svetlov and N. B. Yaremenko, Theory and Properties of Industrial Explosives [in Russian], Nedra, Moscow (1973).
- 9. R. Miller, "Approximate equations of state of detonation products," in: Detonation and Two-Phase Flow [Russian translation], Mir, Moscow (1966).