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A DETONATION WAVE, STATIONARILY PROPAGATED IN CONDENSED
EXPLOSIVES, AND THE EQUATION OF STATE OF THE EXPLOSION PRODUCTS

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-USSR-

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CALCULATION OF THE CHARACTERISTICS OF A
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IN CONDENSED EXPLOSIVES, AND THE EQUATION
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Following is a translation of the article entitled "K raschetu kharakteristik detonatsionnoy volny, statsionarno rasprostranyayushcheysya v kondensirovannykh vv, i uravneniyu sostoyaniya produktov vzryva" (English version above) by S. B. Ratner, in Doklady Akademii Nauk SSSR (Reports of the Academy of Sciences, USSR), Vol XLVIII, No 3, Moscow, 1945, pages 198-201.

(Submitted by Academician N. N. Semenov
on 13 October 1944.)

1. In order to determine four characteristics of the detonation wave, that is, the velocity D of the detonation, the velocity U of the explosion products immediately ahead of the front, their density $\rho = 1/v$ and the pressure p in the front, the hydrodynamic theory of detonation provides three laws of conservation (mass, motion, and energy) and the Jouguet-Kryussar condition

$$D = U + C = v_0 \sqrt{-(\partial p / \partial v)_s}, \quad (1)$$

which indicates that the velocity of detonation is equal to the velocity C of sound, relative to the explosion products. As we are not studying the mechanism of detonation for condensed explosive substances, we will consider condition (1) as applicable. The use of limitations in the conservation laws is not required.

The introduction of the equation of state of the explosion products, necessary to determine the isentropic

derivative of pressure with respect to volume, which derivative arises out of condition (1), enables us to find a fifth characteristic: the detonation temperature T . The application of Clapeyron's equation for the explosion products yields:

$$D_{id} = \frac{k+1}{\sqrt{k}} \sqrt{\frac{n}{M} R \sqrt{T}} \approx \frac{\sqrt{T}}{30} \quad (\text{km/sec}), \quad (2)$$

since $k = c_p/c_v \approx 1.2$, and the quantity M/n is the average molecular weight of the explosion products (which products consist, for many explosive substances, of mainly CO_2 , H_2O , N_2 , and CO) may be taken as equal to 30 gm. Inasmuch as T usually equals $3000\text{--}5000^\circ$, then the detonation is close to 2 km/sec; as follows from (2), it is not dependent on the density.

However, it has been observed that the increase of the detonation velocity with density may reach, for explosive substances, a value of 8 km/sec. This is related to the fact that its value is substantially affected by the departure from ideality of the products of explosion, whose density may reach 2 gm/cm^3 . For liquid and solid explosive substances the calculation may be carried out with the use of the equation of state that sets forth the explosion products accurately. Moreover, all formulas relating detonation wave parameters to temperature are altered.

2. One of the first attempts (1916) towards such a type of calculation (applicable to nitroglycerine and to mercury fulminate) was Becker's (1). He set forth the equation of state for nitrogen

$$p = RT\rho(1 + f\rho^{10}) + a\rho^2(n\rho^8 - 1), \quad (3)$$

which corresponds [See Note] to the experimental data of Bridgeman (2), obtained at 65°C for densities up to 1.1 gm/cm^3 . The use of this specific equation is invalid, since it is impossible to identify the explosion products associated with nitrogen, especially when considering the higher density of the explosion products.

[Note] We note that the members of formula (3) which are temperature-independent include an item having a positive value, that is related to the forces of repulsion, and that is predominant over the temperature-dependent members at densities close to 2 gm/cm^3 . Here, and further on, we have in mind the elastic forces of repulsion

against which work is done, since they exert an influence according to $(\partial E/\partial p)_T$. These forces are distinguished from those repulsion forces usually associated with the co-volume, which are of a thermal character. The calculation of the formulas that follow, (4) and (6), does not change the expression $(\partial E/\partial p)_T$, which remains equal to zero, as in the case of Clapeyron's equation.)

Obviously, these circumstances, which are aggravating in that the expression (3) complicates the mathematical computation, led to the fact that Becker's paper stands alone in the literature.

3. A significantly greater development has been evident in an opposite approach, which was chosen somewhat earlier (1912). Taffanel and Dautriche (3), who were supported by Jouguet (4), and then by Schmidt (5) (1935-1936).

They assumed an equation of state in the general form of

$$p(v - \alpha) = \frac{n}{M} RT \quad (4)$$

and, regarding the co-volume as constant, they obtained [See Note] from hydrodynamic theory

$$D = \frac{k+1}{\sqrt{k}} \sqrt{\frac{n}{M} RT} \frac{1}{1 - \alpha \rho_0} = D_{id} \frac{v_0}{v_0 - \alpha} \quad (5)$$

Inasmuch as the calculation of D_{id} is possible from formula (2), these authors suggest that the calculation of D on the basis of the experimental data for the dependence of D on the initial density $\rho_0 = 1/v_0$, which quantity is also to be used for further inter- and extrapolation (3), and also for calculations of detonation velocity for other explosive substances (5).

[Note] The analogous formula (6) had been already obtained in 1891 by Vieille (6), who employed equation (4) in the La Place formula, which relates the expansibility of the gas to the speed of sound, which formula he also adapted to the detonation velocity.)

However, calculations carried out for dynamite (3), trotyl, ten [?], and other substances (5) indicated that the co-volume is not constant: it increases with increasing specific volume. Consequently, the use of $\alpha = \text{constant}$ in the substitution of (4) in (1) is incorrect [See Note] for the detonation of condensed explosive substances,

since the formulas of Taffanel-Dautriche-Schmidt have proven to be inaccurate.

(Note We are indebted for this error to Prof Ya. B. Zel'dovich, who brought it to our attention.)

4. In order to correctly implement the concept of Taffanel and Dautriche, one must select such a form for the equation of state for the explosion products that corresponds to the experimental facts. We employed for this purpose Bridgeman's data (2) as mentioned in paragraph two. These data indicate the possibility of applying equation (4) in the study of the density range of the data, if there is introduced for the co-volume a simbat ya [?] dependence on the volume. We adopted for this dependence the well-known form of van Laar, $\alpha = bv/(c+v)$, transforming (4) into the form of

$$p = \frac{n}{M} RT \frac{v+c}{v\sqrt{v-(b-c)}}, \quad (6)$$

where $b > c > 0$. It is also necessary to determine the last constants from experimental data for $D = D(\rho_0)$.

5. The introduction of formula (6) in the basic equations was carried out differently from the relations established earlier. For U there is obtained

$$U = \sqrt{\frac{nRT}{Mk \left\{ 1 - \frac{bc}{k(v+c)^2} \right\}}} = \frac{(U)_\alpha = \text{constant}}{\sqrt{1 - \frac{bc}{k(v+c)^2}}}, \quad (7)$$

where $U_\alpha = \text{constant}$ corresponds to paragraph four.

Formula (5) is substituted in a system of two equations:

$$D = D_{id} \frac{\sqrt{k} x}{k+1 \sqrt{y(v-b+c)}}, \quad (8)$$

$$v_0 = v \frac{x}{y}, \quad (9)$$

where $x = (k+1)v^2 + \sqrt{2}(k+1)c - b\sqrt{v} + \sqrt{(k+1)c - 2b/c}$; and $y = kv^2 + 2kcv + (kc - b)c$.

This system has a cumbersome algebraic solution (considering the form of x and of y), although in principle it very easily relates (through the parameter v) D

to v_0 , which is very substantial because the relation between them is given by experiment.

6. In order to indicate the numerical deviation that was introduced by Schmidt's error, we -- working with ten [?] -- selected the original data of Schmidt: $k = 1.2$; $M/n = 29.2$ gm; $T = 5000^\circ$ K; $D_{10} = 2.4$ km/sec, and the results that were used by him from the experiments of Fridrikh for $D = D(v_0)$. Solving the system of equations (8) - (9) graphically, we obtained $b = 1.6$ cm³/gm; and $c = 1.36$ cm³/gm. From this the equation of state for the explosion products of ten is

$$p(\text{atm}) = 83.1 \frac{n}{M} \frac{v + 1.36}{v - 0.24} T. \quad (10)$$

As a result, in place of the constant value of $U = 1.09$ km/sec that Schmidt obtained we have in a diapason [may mean range or compass/ of 0.25-1.6 gm/cm³ an increase of U from 1.16 to 1.6 km/sec. For the pressure in the front our results are substituted in the same ratios that were obtained by Schmidt (in particular, at $\rho_0 = 1.2$, the pressure was 82,000 atm according to Schmidt, while for us it was 114,000 atm). An analogous situation exists also in the case of the other parameters.

7. In order to arrive at a conclusion concerning the limits of applicability of the formulas that we obtained, it was necessary to compare the results of the application of these formulas with the direct experimental data (Bridgeman). The results of the comparison (for nitrogen) are shown in the table.

$v \frac{\text{cm}^3}{\text{gm}}$	$p \cdot 10^{-3}$ atm	
	Experiments of Bridgeman (2)	Calculation by Formula (8)
1.29	3	1.97
1.09	6	2.63
0.98	10	3.22
0.91	15	3.75

The nature of the data deviation confirms the role, already reflected in Becker's formula (3), of the temperature-independent forces of repulsion that increase with the density. In such a fashion, adopting for our

calculations the form of the equation of state $p = RT\rho(v)$, it is not possible to reflect the properties of the explosion products at high initial densities of the explosive substances.

8. In the meantime, the employment of precisely this form has opened up the prospect for a complete calculation of the characteristics of the detonation wave in condensed explosive substances, since it established a link between these and the gases, for which the calculation exhibited only surmountable difficulties, as was shown by Zel'dovich and the author (7).

From this follows not only the invalid formulas and calculations of Taffanel-Dautriche-Schmidt, but also the impracticable idea of theirs: to employ the correction coefficient D/D_{id} for the non-ideality of the explosion products.

In order to obtain a correct relation between the quantities which characterize the detonation wave, it is necessary [See Note] to utilize an equation of state that considers the forces of repulsion.

[Note] For this condition we are indebted to Prof L. D. Landau.)

9. Along with these conclusions, inasmuch as the explosion products for the specific classes of explosive substances are similar in composition, it may be assumed -- within the limits of these classes -- that the temperature component of the pressure will be changed to a small extent at a given density. This affords the possibility of utilizing the calculation methods developed, in particular, in application to liquids.

Conclusion. 1. In the utilization of the general equations of the hydrodynamic theory of detonation for condensed explosive substances there has been presented a critique of the preceding studies: those by Becker, Taffanel and Dautriche, Jouguet, and Schmidt.

2. The equations of the hydrodynamic theory are solved with the help of the equation of state of van der Waals, which contains the co-volume in the van Laar form.

3. The calculated constants of the equation of state for the explosion products arises from the experimentally based dependence of the detonation velocity of ten [?] on the density.

4. A reverse comparison with the experimental data of Bridgeman indicates the necessity for a calculation at high densities, where the forces of repulsion are not temperature-dependent.

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