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1962

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PHYSICAL CHEMISTRY

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CALCULATION OF THE PARAMETERS OF DETONATION WAVES OF CONDENSED EXPLOSIVES

(Presented by Academician Ya. B. Zel' dovich on 4 V 1962)

Numerous studies have been devoted to obtaining equations of state for explosion products (e.p.) of condensed explosives (the bibliography is given in ([1])). In most of these works, the parameters entering into the equation of state are determined from experimental data directly on detonation. Such calculations, although they give values of detonation parameters that agree with the experimental ones, have their drawbacks. First, the complexity of the detonation process requires the introduction into the equation of state of e.p. of a large number of parameters, which makes their physical interpretation difficult. Second, the application of empirical or semiempirical equations obtained in this way is limited to the range of explosives whose experimental characteristics were used in choosing the equation of state.

Attempts at an independent calculation of detonation parameters, without recourse to experimental material on the study of detonation waves, as a rule led ([2]) to results differing substantially from experiment. Dynamic methods developed in recent years for studying the compressibility of various substances have made it possible to study, by independent means, the shock compressibility of the main components of e.p.: H_2O ([3], [4]); N_2 and CO_2 ([5]), C (graphite) ([6]). Moreover, for the substances listed the equations of state may also be regarded as established ([5], [6], [8]).

These data characterize the behavior of e.p. in the range of pressures and temperatures of interest to us and remove the principal obstacle to an independent calculation of the characteristics of detonation waves.

Equations of state of the components of e.p.

In the detonation of ordinary high explosives, the main explosion products may be taken to be H_2O, CO_2, N_2, C, CO, and H_2. Nitrogen oxides and certain other compounds found in e.p. apparently cannot play a determining role, owing to their small amounts. The shock compressibility which, under certain assumptions, makes it possible to establish an equation of state is known for all the substances listed, with the exception of CO and H_2.

In passing from shock compressibility to an equation of state for all substances* whose data were used in the calculations of detonation parameters, the conclusions of the Lennard-Jones theory were used (see, for example, (9)). The experimental shock adiabats served for the selection of the parameters of the pair-interaction potential. The results obtained in (5) for the case of a power potential $(9 \div 6)$** were supplemented by analogous calculations for the interaction potential (6-exp)

$$\varphi(r) = \frac{\varepsilon_m}{1 - 6/\alpha} \left[\frac{6}{\alpha} e^{\alpha(1 - r/r_m)} - \left(\frac{r_m}{r} \right)^6 \right], \tag{1}$$

where ε_m is the minimum energy when the particles are at a distance r_m, α is the steepness of the repulsion. r_m is related to the collision parameter r_0 by the equation $\varphi(r_0) = 0$. In contrast to calculations with the power potential $(9 \div 6)$, for the case (6-exp) only the nearest layer of molecules was taken into account in the calculations, as was done originally by the authors of this theory (10). The selection of parameters from experimental adiabats compensated both for the errors thereby allowed and for inaccuracies due to other factors not taken into account by cell theories (nonsphericity of molecules, etc.).

Table 1

Substance	$9 \div 6$: $\frac{\varepsilon_m}{k}$, °K	$9 \div 6$: r_0, Å	(6-exp), $\alpha = 12$: α	(6-exp), $\alpha = 12$: $\frac{\varepsilon_m}{k}$, °K	(6-exp), $\alpha = 12$: r_m, Å	(6-exp), $\alpha = 12$: r_0, Å
N_2	91.6	3.66	12	168	4.16	3.64
CO_2	375*	3.71	12	506	4.21	3.69
H_2O	91.5	3.16	12	117	3.62	3.17

* In (5) the value

$$\frac{\varepsilon_m}{k} = 290^\circ$$

was erroneously given from intermediate calculations.

The parameters of the power potential $(9 \div 6)$ and of the potential (6-exp), selected from shock adiabats, are given in Table 1. The calculated shock adiabats with the choice of the potential (6-exp) as a whole describe the experiment better than the power potential $(9 \div 6)$.

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* With the exception of Pb and C (graphite). For them the equations of state were adopted from (6,7).

** The numbers $(9 \div 6)$ mean that the repulsion energy in the interaction potential is $\sim r^{-9}$, and the attraction energy is $\sim r^{-6}$.

Figure 1. Dependence of the detonation velocity on the initial density of lead azide (a) and mercury fulminate (b). Points are experiment $^{(13)}$.

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Equation of state of the detonation products and results of calculating the parameters of detonation waves

In going from the established properties of the individual components to the equation of state of the detonation products, two assumptions were made.

First, it was assumed that for a mixture of components taken at identical pressures (P) and temperatures (T), in amounts corresponding to their equilibrium composition, the volume and internal energy can be obtained additively from the corresponding quantities for the components.

Second, the assumption concerns the composition of the detonation products. It is assumed that during detonation of condensed explosives the composition is established in such a way that the detonation products occupy a minimum volume. Such a choice of the composition of the detonation products roughly takes into account the displacement of chemical equilibrium toward the formation of products occupying a smaller volume. The requirement of minimum volume uniquely determines the composition of the detonation products in the range of pressures and temperatures of interest to us. It follows from it that, in the detonation of explosives with negative and zero oxygen balance, the detonation products must contain only N_2, CO_2, H_2O, and C (graphite).

The introduction of such assumptions and knowledge of the equations of state of the components of the detonation products makes the calculation of detonation characteristics comparatively simple. The dependences $P(v,T)$ and $E(v,T)$, obtained from the additivity rule for the selected composition of the detonation products, make it possible to construct the shock adiabats of the detonation products. From the latter, together with the tangency condition, the detonation velocity and the state parameters at the Jouguet point are determined graphically.

Fig. 1. Dependence of the detonation velocity on the initial density of lead azide (a) and mercury fulminate (b). Points—experiment $^{(13)}$.

Calculated dependences $D(\rho_0)$ for PbN_6 and $Hg(OCN)_2$ are presented in Fig. 1. The large discrepancy between the experimental and calculated curves with decreasing density apparently cannot be explained by the fact that the assumptions made in the calculation are not justified. This is especially clear in the case of PbN_6, the composition of whose products raises no doubts.

Fig. 2. Dependences of the detonation velocity on the initial density of high explosives: TNT (*a*), and RDX (*b*). Points—experiment (^{14}).

The emerging tendency toward agreement between the experimental and calculated values of D with decreasing initial density of mercury fulminate also indicates that, in the case of initiating substances, the reason for the large discrepancy is not connected with the approximate nature of the calculation. Most likely, in the region of the "hump" of the experimental dependence $D(\rho_0)$, the normal detonation regime is disrupted. The possibility of propagation of "undercompressed" detonation waves in explosives with a small critical diameter (detonation transfer through grains) has already been pointed out earlier (^{11}).

The results of calculating the dependences $D(\rho_0)$ for two high explosives are shown in Fig. 2. The discrepancy of the calculated curves with experiment in the case of high explosives is considerably smaller (the maximum deviation at $\rho_0 = 1.0$ g/cm^3 is $\sim 5 \div 8\%$) and may be explained by an incorrect choice of the composition of the detonation products at low initial density of the explosive. At these densities, the formation of large amounts of CO is possible, which should lead to an increase in the calculated values of D. This is illustrated in Fig. 1b, where the calculated dependences are given for the composition of the detonation products in two variants: all carbon is oxidized to CO (curve I) and according to the requirement of minimum volume, when half of the carbon is oxidized to CO_2 (solid curve II).

The calculated parameters of the same explosives and of nitroglycol are given in Table 2.

Table 2

Explosive	ρ_0, g/cm^3	Calculation (B-eq.): P, kbar	Calculation (B-eq.): ρ, g/cm^3	Calculation (B-eq.): T, °K	Experiment: P, kbar	Experiment: ρ, g/cm^3	Experiment: T, °K	Literature source
TNT	1.0	54	1.35	3300	64	1.34	–	(^{14})
TNT	1.3	104	1.76	4250	125	1.77	–	(^{14})
TNT	1.6	177	2.08	3850	205*	2.17*	–	(^{14})
TNT	1.64	–	–	–	177	–	–	(^{6})
RDX	1.0	92	1.42	4970	–	–	–	–
RDX	1.2	128	1.61	4800	152	1.66	5500–	(^{14})
RDX	1.5	218	1.99	4500	249*	2.08*	–5800	(^{14})
RDX	1.8	334	2.36	4080	390*	2.50*	–	(^{15}), (^{14})
RDX	1.8	–	–	–	341	–	–	(^{6})
Nitroglycol**	1.5	200	1.97	5090	–	–	4400 (^{16})	–
Lead azide	2.5	60	3.24	3300	–	–	–	–
Lead azide	3.56	150	4.45	3040	–	–	–	–

Explosive	ρ_0, g/cm^3	Calculation (B-eq.): P, kbar	Calculation (B-eq.): ρ, g/cm^3	Calculation (B-eq.): T, °K	Experiment: P, kbar	Experiment: ρ, g/cm^3	Experiment: T, °K	Literature source
Lead azide	4.0	215	5.00	2800	–	–	–	–
Lead azide	4.8	360	5.88	1850	–	–	–	–
Mercury fulminate	2.0	52	2.89	6320	–	–	–	–
Mercury fulminate	3.56	162	4.78	6260	–	–	–	–
Mercury fulminate	4.0	215	5.25	6200	–	–	–	–
Mercury fulminate	4.41	264	5.66	6000	–	–	–	–

* Values obtained by interpolation.
** $D_{\text{calc}} = 7.50, \quad D_{\text{exp}} = 7.40$ (^{16}).

It should be noted that, for the chosen equation of state of the detonation products, the Jouguet condition determines with sufficient accuracy the slope of the detonation ray and, consequently, the detonation velocity. The position of the tangency point is fixed less accurately, i.e., the parameters P, ρ, T, which are determined by it. Nevertheless, as is evident from comparison with the experimental data (Table 2),

agreement, taking into account the rough nature of the assumptions made in the calculation, may be considered quite satisfactory. A comparison of the two calculation variants, differing in the choice of potential, presented in Figs. 1–3 and in Table 2, shows that the agreement of the calculated quantities is sufficiently good and, consequently, that the errors allowed in determining the equations of state of the components are small.

The authors take this opportunity to express their gratitude to L. V. Al' tshuler and Acad. Ya. B. Zel' dovich for valuable advice and their constant interest in the work, and to N. V. Panov and L. A. Chernova for assistance with the computational work.

Received
7 III 1962

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