FTD-TT- 65-1004

TRANSLATION

CALCULATION OF COMPOSITION OF EXPLOSIVES AND DETONATION PARAMETERS OF CONDENSED EXPLOSIVES

By

V. N. Zubarev and G. S. Telegin

FOREIGN TECHNOLOGY DIVISION

AIR FORCE SYSTEMS COMMAND

WRIGHT-PATTERSON AIR FORCE BASE

OHIO

Code 1

FTD-TT- 65-1004/1+2+4

UNEDITED ROUGH DRAFT TRANSLATION

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English pages: 9

SOURCE: AN SSSR. Doklady. (Russian), Vol. 158, No. 2,
1964, pp. 452-455.

S/0020-064-158-002

TP5002162

	PREPARED BY: TRANSLATION DIVISION FOREIGN TECHNOLOGY DIVISION WP-AFB, OHIO.

FTD-TT- 65-1004/1+2+4

Date 30 Nov. 1965

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CALCULATION OF COMPOSITION OF EXPLOSIVES AND DETONATION PARAMETERS OF CONDENSED EXPLOSIVES

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During the calculation of detonation wave parameters of condensed explosives (1) on the basis of data of dynamic compressibility of components of explosive products (P.V.) (2-4) there was accepted a constant composition of (P.V.) = explosive products, determinable by the requirement of minimum volume. According to this requirement in brisantine explosive products V.V. with negative oxygen balance the formation of CO and H_2 is excluded. This substantially simplifies the calculations, but is justified only at V.V. detonation of greater initial detonation.

In this report the possibility of formation on P.V. of Co and H_2 was considered, the concentration of which, as well as other components were determined from the condition of chemical equilibrium.

Calculation of P.V. composition. At a detonation lay-out of brisantine V.V. in explosion products, discovered during explosions in calorimetric devices, the basic place is taken up by N_2, H_2O, CO_2, H_2 and C (graphite) that is decomposition of V.V. molecules takes place basically according to the system

$$C_aH_{2d}O_bN_{2n} \rightarrow y\,H_2 + (d-y)\,H_2O + x\,CO + + n\,N_2 + \frac{b-d-x+y}{2}\,CO_2 + \frac{2a-b+d-x-y}{2}\,C. \qquad (1)$$

Equations of the state of decomposition products (1) at high pressures are known (1, 4, 5). Carbon oxide by physical properties is very close to N_2 and during its description data can be used from equation of the state of nitrogen (4). About the properties of hydrogen, which is included in P.V. in small amounts, can be judged by calculation data (6).

When changing over from properties of individual components to the equation of the state of P.V. in this report, as well as in (1), there was proposed an additiveness of volumes and internal energies, i. e., to explosion products were ascribed properties of a multicomponent ideal solution.

In the assumption of equilibrium the P.V. composition is determined by conditions of chemical equilibrium. Chemical potentials of gaseous components were determined by the theory of free volumes.

It was considered that carbon is found in P.V. in condensed phase (graphite). Its equation of state and chemical potential was adopted by (5).

During the decomposition of V.V. by formula (1) in explosive products, two independent reactions are possible: 1) $CO_2 + C \rightleftarrows 2CO$ and 2) $CO + H_2O \rightleftarrows CO_2 + H_2$.

Table 1.

1) Kbar P, кбар	K_1					K_2				
	2000° K	3000° K	4000° K	5000° K	6000° K	2000° K	3000° K	4000° K	5000° K	6000° K
50	$3{,}69\cdot 10^{\text{[illegible]}}$	5,34	0,214	$5{,}2\text{[illegible]}\cdot 10^{-\text{[illegible]}}$	$2{,}19\cdot 10^{-\text{[illegible]}}$	8,78	11,8	12,7	13,6	14,3
100	$9{,}27\cdot 10^{\text{[illegible]}}$	18,8	2,16	0,434	0,146	19,3	21,6	18,3	17,8	17,8
200	$6{,}75\cdot 10^{\text{[illegible]}}$	$1{,}61\cdot 10^{\text{[illegible]}}$	33,8	4,41	1,30	$1{,}33\cdot 10^{\text{[illegible]}}$	72,5	45,8	37,0	29,3
400	$3{,}01\cdot 10^{\text{[illegible]}}$	$1{,}31\cdot 10^{\text{[illegible]}}$	$9{,}74\cdot 10^{\text{[illegible]}}$	87,7	14,4	$4{,}22\cdot 10^{3}$	$7{,}17\cdot 10^{\text{[illegible]}}$	$2{,}61\cdot 10^{\text{[illegible]}}$	$1{,}36\cdot 10^{\text{[illegible]}}$	94.5
600	$1{,}57\cdot 10^{10}$	$2{,}44\cdot 10^{\text{[illegible]}}$	$1{,}14\cdot 10^{\text{[illegible]}}$	$7{,}00\cdot 10^{\text{[illegible]}}$	$1{,}14\cdot 10^{\text{[illegible]}}$	$1{,}34\cdot 10^{\text{[illegible]}}$	$6{,}11\cdot 10^{\text{[illegible]}}$	$1{,}17\cdot 10^{\text{[illegible]}}$	[illegible]	

1) P, Kbar

Some calculated values of equilibrium constants of these reactions are given in Table 1, from which it is evident that both constants depend sharply upon pressure. This dependence is due basically to the presence in constants K of a co-factor $e^{P}\,\Delta v/RT$ (Δv change of substance during reaction), which at high pressures $\sim 10^5$ atm begins playing a decisive role, displacing directions of reactions in the direction of products with smaller volume.

At relatively small pressures the reaction equilibrium constant of generator gas depends upon pressure in a trivial way, since $K_1 \sim \frac{v_0(P_0,T)}{v(P,T)}\, e\, \frac{\Delta\Phi}{RT}$ which for an ideal gas is equivalent to $K_1 \sim \frac{P}{P_0}\, e - \frac{\Delta\Phi}{RT}$. An increase in $K_1 \sim$ by 10^5 times at a change in pressure from 1 atm to 10^4 atm takes place mainly on account of this linear dependence upon pressure. At much higher pressures the ratio v_0/v changes relatively weakly and the value K_1 is determined basically by the expotential co-factor.

Equilibrium constants K_1 and K_2 determine the amount of CO and H_2 in explosion products and concentration of remaining P.V. components. In case of oxidation of the entire oxygen, i. e., $x + y = 2a + d - b$, the amounts of CO and H_2 in P.V. are situated, in accordance with this condition, by the known value K_2.

The relative number of Co, H_2 moles in explosion products is shown in Figure 1. Concentration of CO, as is evident from graph, Figure 1a, at a pressure of ~300 kbar and temperature of 4000°K is small, but rises sharply at a pressure reduction. From Figure 1b, it is evident that the formation of hydrogen at V.V. detonation of greater initial density can be practically disregarded in all cases.

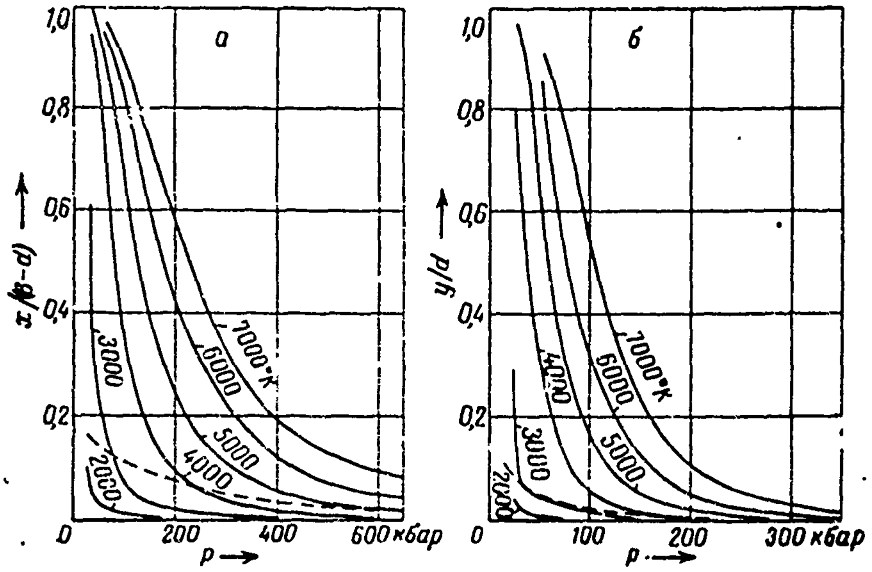

Figure 1. Dependence of CO (a) and H_2 (b) concentrations upon pressure and temperature. When formulating curves a, the formation of H_2 in P.V. was not considered.

Results of calculating detonation wave parameters. Equation of P.V. state in table form in the range of pressures ranging from 25 to 650 kbar and temperatures up to 7000°K were compiled for five most propagated brisantine V.V.: TNT, Hexogene, TEN, tetral and picric acid. The obtained data were used for the calculation of parameters of normal detonation waves by a conventional method with the use of Zhuge conditions.

Some calculation results are given in Table 2. For illustration in Figure 2 is given a comparison of calculated dependences $D(\rho_o)$ with the experiment for two most investigated C.C.: trotyl and hexogene. As is evident from the comparison, calculated dependences practically coincide with experimental data. Calculated rates of detonation and other investigated V.V. also do not differ from the experimental by more than 3%.

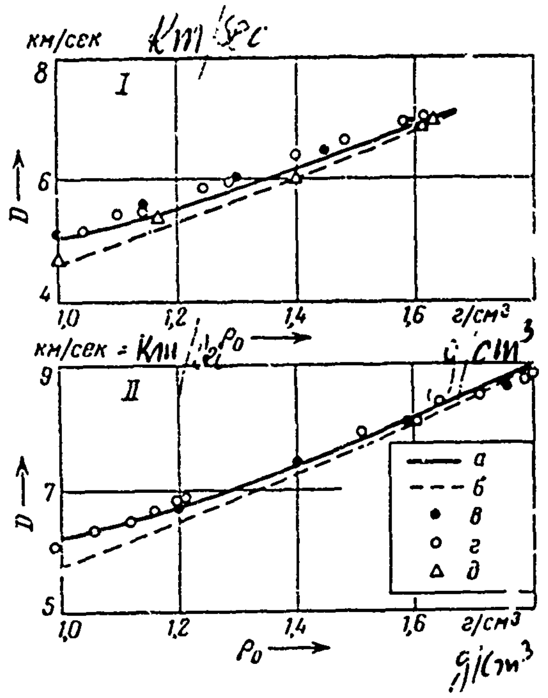

Figure 2. Comparison of calculated dependences D($_o$) with experimental data for trotyl (I) and hexogene (II).
a) calculation of given work; b) calculation with constant P.V. composition (1). Experimental points: v-by (7); g-by (10), d-by (11).

Good conformity of calculated and experimental rates of detonation for many V.V. at different initial densities confirms the correctness of determining equations of state of P.V., and consequently attest to the thing that the additiveness laws adopted in the calculations and the chemical equilibrium conditions of P.V. are fulfilled sufficiently well.

In addition, the satisfactory conformity of calculation and experiment proves that the measured in experiments rates of detonation correspond (or are at least close) to the Zhuge condition. We will mention that the correctness of this confirmation was in doubt in certain calculations (12).

When comparing calculated pressures with experimental, there is discovered a considerably greater difference than in the rates of detonation. The divergence in some cases reaches 10-15%. These differences can be combined with greater sensitivity of tangent point position to the process of shock adiabates P.V. It is sufficient to mention that at a change in pressure on the adiabate by 1 - 2%, the displacement of the tangent point may lead to a change in Zhuge pressure by 10% and more.

Some values were obtained by extrapolation or interpolation of experimental data. The relative high temperatures of P.V. (Table 2) appe appear to be the main result of the thing, that the realizing of detonation of dense V.V. calculated composition of P.V. corresponds practically to the maximum calorific, which by much exceeds the heat of explosion, measured in calorimetric bombs (see for example (13). This is explained by the fact, that at more considerable degrees of expansion of P.V. in calorimetric devices there is observed a substantially greater concentration of CO, than given by calculation at high pressures.

Table 2.

В. в.	Расчет 1)				Эксперимент * 2)				
	v_0, см³/г	D, км/сек km/sec	P, кбар kbar	T, °K	v_0, см³/г	D, км/сек	P, кбар Kbar	T, °K	Источник Source
ТНТ TNT	1,0	5,01	73	3870	1,0	5,1	66,2	—	(7)
	0,8	5,67	105	3830	0,8	5,88	113	—	(7)
	0,610	7,04	184	3740	0,610	6,94	189	—	(8)
						7,00	212		(8)
Гексоген Hexogene	1,0	6,22	104	4560	1,0	6,05	104	—	(7)
	0,8	6,84	153	4540	0,8	6,92	166	—	(7)
	0,6	8,46	250	4200	0,6	8,36	322	—	(7)
	0,555	9,00	340	4000	0,555	8,77	354	—	(8)
						8,85	392	3700	(8)
ТЭН TEN	1,0	5,70	88	4850					
	0,8	6,72	150	4780					
	0,6	8,16	270	4500					
	0,565	8,61	310	4400	0,565	8,50	342	4200	(8)
Тетрил Tetryl	1,0	5,20	75	4000					
	0,8	5,98	115	4000					
	0,588	7,80	250	4000	0,588	7,85	283	2950	(8)
Пикриновая кислота Picric acid	1,0	5,32	84	4120	1,0	5,22	—	—	(10)
	0,8	5,93	117	4100	0,8	6,07	—	—	(10)
	0,6	7,30	200	4070	0,6	7,34	—	—	(10)

1) calculation; 2) experiments

From this viewpoint it is interesting to investigate the change in composition of P.V. at their izentropic expansion. Calculation at pressures of 25 - 300 kbar and the temperature of $2.10^3 \div 4.10^{3}$°K, shows that $\left(\frac{\partial \ln P}{\partial \ln T}\right)_s$ changes in relatively narrow limits from 4 to 6. Assuming approximately, that on the izentropy of P.V. $P \sim T^5$ can be presented an approximate process of changes in composition at expansion of P.V, which is shown in Figure 1 (dotted lines). At a reduction in pressure in the izentropy of P.V. there is an increase in the amount of CO and H_2, which qualitatively explains the difference in experimental and calculated data about the composition of P.V.

The calculations made of the composition of P.V. qualitatively explain also the experimental fact of reducing the heat of explosion at a reduction of the initial density of V.V. (14). According to data in Table 2, the temperature of P.V. remains practically unchanges, and the greater change in pressure leads to a displacement of reactions 1 and 2 to the right, e.i., to a reduction of the separating chemical energy.

In conclusion we will mention, that sufficiently correct qualitatively conclusions about equations of state of P.V. for the calculation of composition of P.V. and detonation characteristics was found to be possible to make thanks to the presence of data about the components of e explosive products at high pressures. Investigation of dynamic compressibility of individual components of P.V. which began with the study of shock adiabate of water (2) and continued during the measurement of dynamic compressibility of N_2 and CO_2 (4) gave highly valuable data, which allow by properties of a relatively small number of components to determine the characteristics of detonation waves of numerous brisant V.V.

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