TRANSLATION

CALCULATION OF COMPOSITION OF EXPLOSIVES AND DETONATION PARAMETERS OF CONDENSED EXPLOSIVES

By

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English pages: 9

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CALCULATION OF COMPOSITION OF EXPLOSIVES AND DETONATION PARAMETERS OF CONDENSED EXPLOSIVES

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V. N. Zubarev, G. S. Telegin

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 bris-antine explosive products V.V. with negative oxygen balance the formation of CO and \( \text{H}_2 \) 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 \( \text{H}_2 \) 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 bris-antine V.V. in explosion products, discovered during explosions in calorimetric devices, the basic place is taken up by \( \text{N}_2 \), \( \text{N}_2\text{O} \), \( \text{CO}_2 \), \( \text{H}_2 \) and \( \text{C} \) (graphite) that is decomposition of V.V. molecules takes place basically according to the system

\[ \text{PTD-TT-65-1004/1+2+4} \]
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 volume.

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$\rightleftharpoons$ 2CO and 2) CO + H$_2$O$\rightleftharpoons$ CO$_2$ + H$_2$.

FTD-TT-65-1004/1+2+4 2
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 $e^D \Delta v/RT$ ($\Delta v$ 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 $K_1 \sim \frac{\nu_0(P_0,T)}{\nu(P,T)} e^{\Delta \frac{\phi}{RT}}$ which for an ideal gas is equivalent to $K_1 = e^{\frac{\Delta \phi}{RT}}$.

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 $\nu_0/\nu$ changes relatively weakly and the value $K_1$ is determined basically by the exponential co-factor.

<table>
<thead>
<tr>
<th>$P$, Kbar</th>
<th>$K_1$</th>
<th>$K_2$</th>
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<tr>
<td>50</td>
<td>3.05-10^4</td>
<td>5.34</td>
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<td>100</td>
<td>7.27-10^4</td>
<td>10.8</td>
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<td>6.75-10^4</td>
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<td>500</td>
<td>3.04-10^4</td>
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<tr>
<td>600</td>
<td>1.57-10^4</td>
<td>2.44-10^4</td>
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</table>

1) $P$, Kbar

**Table 1.**
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

![Figure 1](image.png)

**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.

a pressure of \( \sim 300 \) kbar and temperature of 4000\(^\circ\)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.

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\(^\circ\)K were compiled for five most propagated brisant-
tine 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 $D\left(\phi_0\right)$ 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 $D\left(\phi_0\right)$ with experimental data for trotyl (I) and hexogene (II).

a) calculation of given work; b) calculation with constant P.V. composition (I). 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 adiabats 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) 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

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

6
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.

<table>
<thead>
<tr>
<th></th>
<th>Расчет 1)</th>
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<td>к. в.</td>
<td>Т.</td>
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1) расчет; 2) эксперимент

From this viewpoint it is interesting to investigate the change in composition of P.V. at their isentropic expansion. Calculation at pressures of 25 - 300 kbar and the temperature of $2.10^3 \div 4.10^3 K$, shows that $\frac{\partial}{\partial T} \ln \left( \frac{P}{T} \right)$ changes in relatively narrow limits from 4 to 6. Assuming approximately, that on the isentropy 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 isentropy of P.V. there is an increase in the amount of CO and H$_2$, which qualitatively explains the difference

PTD-TT-65-1004/1±2±4 7
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 unchanged, 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 N₂ and CO₂ (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.
Literature


