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EVALUATION OF ENERGY AND PERFORMANCE OF EXPLOSIVES

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The paper presents an analysis of problems of evaluation of the energy content and performance of high explosives. A description is mentioned of the Cylinder test as a modern experimental method for obtaining more complex and versatile information necessary for this evaluation. The calculations from JWL state equation have been used to document differences in mechanisms of energy release by various explosives during detonation.

Introduction

While planning a synthesis of individual explosives or preparation of new energetic compositions, we almost always encounter the question of how they will differ in their character from known explosives. Such a comparison has a fundamental aspect in evaluation of energy and performance, and it is generally requested to maintain or increase these characteristics. The increase in these

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parameters is routinely represented in percents referenced to a chosen standard. Most often, such a standard is trinitrotoluene (T.N.T.) or its mixture with hexogen (RDX) in the RDX/T.N.T. mass ratio equal to 60/40.

The evaluation performed in this way, of course, is highly questionable for many reasons: the energy and also performance parameters can be defined, expressed, calculated and also experimentally determined in different ways. It appears that for the used performance parameters and cognate relationships to possess a sufficient predicative ability it is necessary that they should be described in more detail, inclusive of giving the description of the experimental method used for their verification.

Theory

In order to better understand the meaning of different parameters and their relationships, let us start from the basic idea of explosive conversion of high explosives. High explosives commonly release their energy by detonation, which produces a detonation shock wave and products (usually highly compressed and very hot gases). Hence, this process is characterised by detonation and energy parameters.

Detonation Parameters

Basic detonation parameters of explosives include the following:

- detonation velocity D (in $\mathrm{m\,s^{-1}}$)
- detonation pressure P (in GPa)
- detonation energy E_D (in $\mathrm{kJ\,g^{-1}}$ or $\mathrm{MJ\,kg^{-1}}$)

These quantities — particularly the detonation velocity and pressure — directly depend on the density of explosives ρ (in $\mathrm{g\,cm^{-3}}$). With increasing density of a given explosive its detonation velocity grows linearly (or almost linearly), whereas the pressure and energy grow with the square of density.

For the above-mentioned parameters we can write the following relationships [1]

$$P = \frac{\rho D^2}{\gamma + 1} \tag{1}$$

$$E_D = \frac{D^2}{2(\gamma^2 - 1)} \tag{2}$$

$$E_D = \frac{P}{2(\gamma - 1)}\rho \tag{3}$$

where γ is adiabatic exponent, which is defined from the pressure-volume relation (at constant entropy) for adiabatic expansion of gaseous products of detonation. Under these conditions it can be calculated from the equation

$$\gamma = \rho\frac{D^2}{P} - 1 \tag{4}$$

If we introduce D in km s^{-1}, ρ in g cm^{-3} and P in GPa, then the γ values for different explosives will vary within the interval of 2.50 – 3.30.

Energy Parameters

Three kinds of energy are distinguished when evaluating the energy content of explosives [2]:

- detonation energy E_D, which is necessary for a stable course of detonation
- compression energy E_C, which is present in the gaseous detonation products in the original volume of charge
- total energy E, which can be released by the explosive in its detonation conversion. This energy is the sum of the detonation and compression energies

$$E = E_D + E_C \tag{5}$$

We can determine this total energy from the difference between heat of formation of detonation products, H_{fi}, and heat of formation of the explosive, $H_{f,ex}$

$$E = \frac{\sum H_{fi} - H_{f,ex}}{\text{molecular weight}} \tag{6}$$

The compression energy E_C can be calculated [2] by modifying Eqs (2) – (6) into the form of

$$E_C = E - \frac{D^2}{2(\gamma^2 - 1)} \tag{7}$$

$$E_C = E - \frac{P}{2(\gamma - 1)}\rho \tag{8}$$

Equations of State

The behaviour of detonation products is generally described by the equations of state [6].

At present, the expansion of products is usually described by means of the JWL equation of state in the form of Eq. (9)

$$p_S = Ae^{-R_1 V} + Be^{-R_2 V} + CV^{-(\omega+1)} \tag{9}$$

where p_S is pressure of products for a defined expansion (pressure related to a given volume of detonation products), A, B and C are linear constants (in the dimension of detonation pressure), R_1, R_2 and ω are non-linear and non-dimensional coefficients, and V is the relative volume of detonation products (related to the original volume of explosive).

Experimental Verification of Parameters

For the calculation of the above-mentioned parameters to be possible it is sufficient to know the detonation velocity and pressure for a given density of charge. Both the values for a given explosive can be calculated, e.g., from Kamlet's equations on the basis of knowledge of the composition, heats of formation, and densities of the explosives [3,4].

At present, for experimental verification of the calculated parameters it is possible to use a variety of different experimental methods. The methods adopted

can be very specialised but on the other hand, also relatively complex and versatile. Also the accuracy and reliability of the individual methods plays a considerable role. For example, even the relatively simple and, at present, already excellently mastered measurement of detonation velocity (as one of the basic detonation parameters) is considerably affected by experimental conditions, which have to be taken into account in evaluation of these methods. Even more complicated is the problem of measurement of the detonation pressure as an absolutely fundamental performance parameter in relation to deformation as well as acceleration ability of explosives. Therefore, at the present conditions the versatile tests based on practically useful application principles are becoming increasingly preferred. Nowadays, it is considered that the most valuable methods are those that come from indirect determination of performance parameters. They include, first of all, the Aquarium tests and Cylinder test, which start from derivation of performance parameters from measured energies of accelerated materials. The possibility of obtaining reliable outputs while maintaining reasonable demands on the part of the testing and evaluating process is the main reason of their wide application, especially that of the Cylinder test.

Cylinder Test (C.T.) [5]

As it was mentioned above, the C.T. method is a measuring and testing method based on the principle of evaluation of energy of the mass accelerated by explosion. An orientation scheme of arrangement and function of the charge for C.T. is given in Fig. 1.

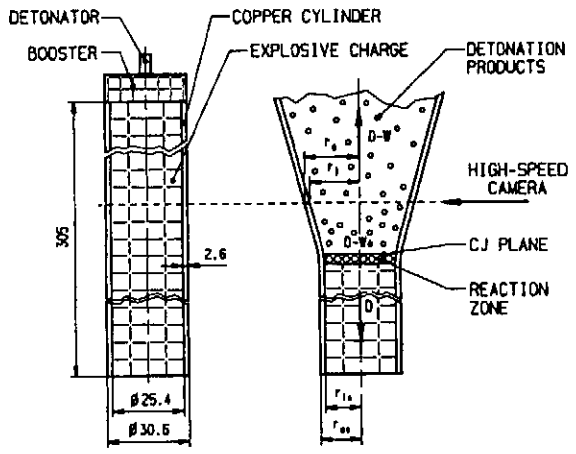

Fig. 1 Scheme of charge and its function in C.T.

This test provides valuable information about quality of investigated explosives regarding their real working ability in a given arrangement, which is closely modelling the most common applications. In addition, this method can be used to test (with only small exceptions) a variety of known (not only brisant) explosives with taking into account potential construction limitations.

The principle of C.T consists in evaluation of optical record of acceleration of the fragmenting wall of the metal case in which the tested explosive had been placed.

During the experiment, the test set is placed in the record area of a recording optical device (for a scheme of measuring arrangement, see Fig. 2), which is able to record the very quickly proceeding actions (the recording frequency is in microseconds). Basically, two kinds of this equipment are predominantly used: ultra-rapid optical cameras or flash X-ray apparatus. Examples of typical resulting records are given in pictures [6] (Fig. 3 presents an optical record, Fig. 4 gives an X-ray record).

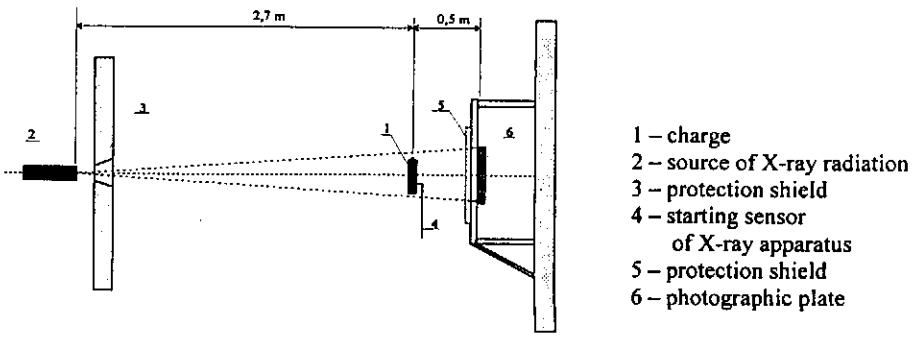

Fig. 2 Scheme of equipment for measuring the C.T with help of flash X-ray apparatus

The obtained test record (i.e. scattering of the case as a result of expansion of detonation products) forms a basis for construction of the so-called expansion curve (i.e. the time dependence of outer diameter of expanding case ($2r_a$)). In principle, this dependence reflects the shape of the case-surrounding boundary, and it is processed by means of specialised graphical and subsequently numerical computerised applications [7].

There are a number of possible processes for mathematical expression of expansion of the case and/or its acceleration. At present mostly used are the computerised numerical methods based on various simplifying models in combination with non-linear curve fitting techniques [8].

The overall evaluation of C.T. represents a complicated and computationally rather demanding task, which is performed in several subsequent steps [9,10].

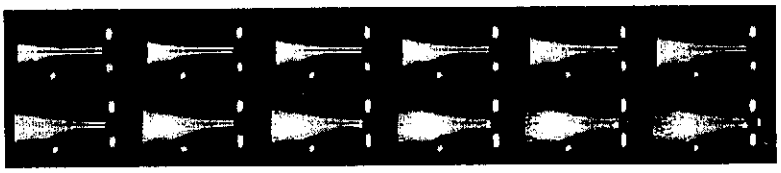

Fig. 3 Optical record of measuring the C.T (French camera of CIAS type)

Fig. 4 Record of measuring the C.T by flash X-ray apparatus (positive)

Process of evaluation of C.T.

- analysis of the obtained expansion curve
  - * determination of parameters of equation expressing the increase in outer diameter of the tube
  - * calculation of radial velocity of the wall
  - * calculation of specific acceleration
- calculation of expansion angle
- calculation of real velocity of the wall and the acceleration
- calculation of the pressure
- calculation of velocity of the particles
- calculation of relative volume $V(v/v_0) = \rho_0/\rho$
- calculation of parameters of JWL equation of state

From the above-described process it clearly follows that, beside the basic output of C.T. (that is derivation of velocity of the wall of expanding case and/or determination of the directly connected value of GURNEY's energy of the explosive tested), the possibilities of evaluation of C.T. are distinctly broader. In this connection, an aspect of fundamental significance for determination of the actual performance of the explosive tested lies in the possibility of determination of JWL coefficients of equation of state, i.e. A, B, C, R_1, R_2 and ω in Eq. (9).

If the respective parameters are known, it is possible — from this equation

Table I Values of energies and detonation parameters of chosen explosives

	ρ, g cm^{-3}	P, GPa	D, m s^{-1}	γ, -1-	E, kJ g^{-1}	E_D, kJ g^{-1}	$E_D/E\times100$, %
A	1.634	26.0	7840	2.862	5.539	4.273	77.1
B	1.672	27.5	8330	3.218	5.673	3.708	65.3
C	1.660	22.0	7600	3.358	7.829	2.810	35.9

Table II Values of JWL parameters of chosen explosives

	A, GPa	B, GPa	C, GPa	R_1	R_2	ω
A	570.2	6.13	1.325	4.45	1.0	0.38
B	950.4	10.98	1.816	5.00	1.4	0.40
C	1341.3	32.70	1.334	6.00	2.0	0.20

Table III Values of the pressure of products of detonation for $V = 1 \div 10$

	$V(v/v_0)$	1	2	3	4	5	6	7	8	9	10
A	P_S, GPa	10.239	1.416	0.597	0.308	0.185	0.127	0.096	0.077	0.065	0.056
B		9.084	1.188	0.438	0.264	0.195	0.156	0.129	0.110	0.096	0.084
C		10.927	1.399	0.555	0.301	0.201	0.150	0.120	0.099	0.084	0.072

of state — to exactly determine (calculate) many important parameters of the given explosive inclusive of the performance parameters.

As compared with other equations of state, the JWL equation of state can be applied, first of all, to hydrodynamic calculations such as numerical simulations etc.

Calculations

In order to more closely explain the relationships between energy of an explosive and its performance, we will make a comparison of parameters for following mixed explosives [1]

A – RDX/ energetic binder in the mass ratio of 75/25
B – HMX/ inert binder in the mass ratio of 88/12
C – RDX/Al/ inert binder in the mass ratio of 64/20/16
where RDX – 1,3,5-trinitro-1,3,5-triazacyclohexane, hexogen

HMX – 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane, octogen
Al – aluminium

From the known values of density ρ, detonation velocity D, and pressure P, and with help of Eqs (2), (4), and (6), we calculated the following quantities for the above-mentioned explosives: adiabatic exponent γ, total energy E, and detonation energy E_D. The results of calculations are presented in Table I.

The values of coefficients of JWL EOS obtained from experimental data [1] are, for the explosives investigated, summarised in Table II. If we introduce these parameters into Eq. (9), we can calculate the values of corresponding pressures of products for various values of expansion — see Table III.

Discussion

When designing or evaluating a new explosive, we can calculate its detonation and energetic parameters from Eqs (1) through (8) given in theoretical part. However, we can see from the data of Table I that, although the total energy increases in the series $A \rightarrow B \rightarrow C$, this trend is not observed with detonation parameters, and it is even opposite for the detonation energy E_D. The main reason of this contradictory behaviour lies in differences between the time dependences of chemical reactions. From this point of view, the detonation zone reactions can be classified as follows: kinetically controlled reactions (usually decomposition of molecules of individual explosives at the level of intramolecular bonds), and reactions controlled by a transfer of mass (in this case, two particles must efficiently collide if they are to react). An example of the latter type of reactions in detonation wave is the reaction of two molecules (oxidiser-fuel), which can be described by a model of collision theory.

The kinetically controlled reactions are distinctly faster: they can proceed almost completely in the reaction zone of detonation wave, which considerably increases the detonation velocity and pressure and also the proportion of detonation energy E_D in the total energy E. The higher is this proportion (E_D/E), the more the detonation approaches to ideal behaviour.

On the other hand, if the detonation reactions are controlled by transfer of mass (by diffusion), then in reaction detonation zone the particles do not manage to finish their reactions, and these reactions are finished as late as in the expanding products. The detonation process is slower, the detonation velocity and pressure are lower, and the proportion of detonation energy is lower too. This means a non-ideal detonation. An example of such behaviour is represented by substances in Table I, particularly substance C, which has a high energy content, but aluminium can only release its energy content within a distinctly longer reaction time than that available in the detonation wave, so it reacts with a delay — as late as in the

expanding products of detonation. By that, the basic parameters of detonation and also the detonation energy itself are markedly decreased.

It is just the application of JWL EOS that can provide a clear illustration of the differences between detonation reactions of individual explosives. If the necessary coefficients of the equation are known (they can be obtained by means of C.T., see Table II), it is possible to calculate the pressures of detonation products at different values of the relative volumes V corresponding to the increasing expansion of detonation products (see Table III).

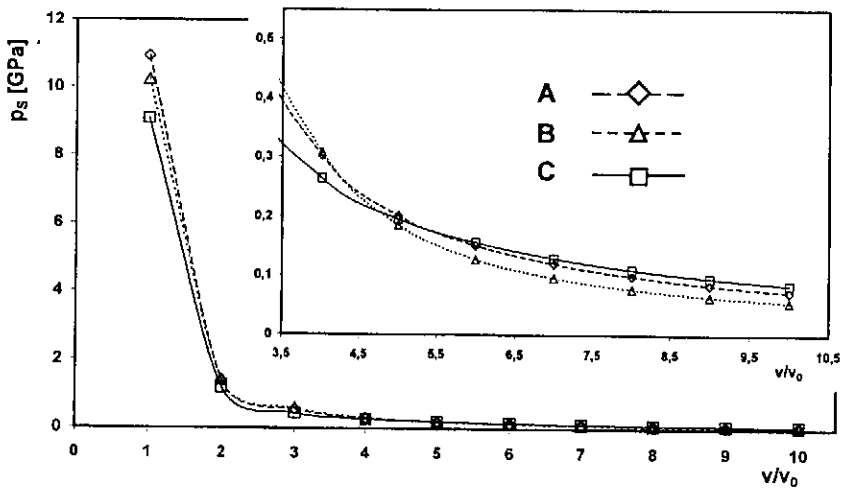

Fig. 5 Graph of dependence of the pressure of products of detonation on their relative volume

The diagram in Fig. 5 shows a rapid decrease in pressure during initial expansion. With continuing expansion this pressure decrease becomes slower. The detail of graph in Fig. 5 schematically illustrates the above-mentioned effect of differences in energy release for different regimes of detonation process. At the relative volume V approximately equal to 5 (i.e. if the volume increases five times in comparison with the original volume of explosive), the aluminium explosive C shows a distinct deceleration of pressure decrease as compared with explosive B and especially A. This is caused by the effect just mentioned, i.e. the effect of different velocities of energy release by the individual components of the explosive in connection with dominant controlling mechanisms of detonation process; in this case they are reactions of aluminium with water and carbon oxides.

Conclusion

Knowing the characteristics and initial detonation parameters — first of all velocity, pressure and original density of an explosive — we can calculate its detonation, compression and total energy. If the ratio of detonation energy to total energy is low, we can expect a longer time course of reactions in the detonation process, which corresponds to non-ideal detonation regime.

A very good experimental method for verification of the calculations is provided by the Cylinder test, which enables sufficiently complex and reliable determination of basic detonation and energetic parameters.

Hence, for evaluation of energy and performance of intended new explosives we have to consider not only important detonation parameters but also energetic parameters including serious appreciation of their real working ability.

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