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Calculation of Detonation Parameters by EXPLO5 Computer Program

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Abstract. Detonation parameters of several high explosives were calculated using own chemical-equilibrium computer program named EXPLO5. The program is based on the chemical equilibrium, steady-state model of detonation. It uses the Becker-Kistiakowsky-Wilson's equation of state (BKW EOS) for gaseous detonation products and Cowan-Fickett's equation of state for solid carbon. The calculation of equilibrium composition of detonation products is done in the program by applying modified White, Johnson, and Dantzig's free energy minimisation technique. The program is designed so that it enables the calculation of detonation parameters at the CJ point, as well as parameters of state along the expansion isentrope.

The paper summarises results of the calculation of the detonation parameters of several standard high explosives by EXPLO5 program, using own set of constants in the BKW equation of state, so-called BKWN set ($\alpha = 0.5$, $\beta = 0.176$, $\kappa = 14.71$, and $\theta = 6620$). It was shown in the paper that the program can be used for the calculation of detonation velocity, pressure, temperature, heat, and detonation energy with reasonable accuracy – these detonation parameters can be calculated with the error less than 10 %.

Introduction

EXPLO5 – an own computer program for the calculation of detonation parameters of explosives is based on the chemical equilibrium, steady-state model of detonation [1]. The program uses the Becker-Kistiakowsky-Wilson (BKW) equation of state based upon a repulsive potential applied to the virial equation of state, to express the state of gaseous detonation products. The BKW equation of state in the following form is used [2]:

$$\frac{pV}{RT} = 1 + xe^{\beta x}; \qquad x = \frac{\kappa \sum X_i k_i}{\left[V(T+\theta)\right]^{\alpha}}. \tag{1}$$

where X_i is mol fraction of i-th gaseous product, k_i is molar covolumes of i-th gaseous product, and α, β, κ, and θ empirical constants.

The free energy minimisation technique, developed by White, Johnson and Dantzig [3], and modified by Mader [2], is applied for the mathematical expression of the equilibrium state of detonation products. The system of equations, formed according to this technique, is solved applying modified Newton's method of the following approximations [4].

The program EXPLO5 calculates the parameters of state of the products along the shock adiabate, starting from a density of a given explosive (ρ_0) and then increasing it in an arbitrary chosen step up to the density of about $1.5 \cdot \rho_0$. Then, it determines the CJ point as a point on the shock adiabate at which the detonation velocity has minimum value. Ones the CJ point was determined the detonation parameters have been calculated applying the well-known relationships between them [1].

The program EXPLO5 also calculates the parameters of state along the expansion isentrope, starting from the CJ point and then increasing specific volume by a selected step up to some desired value (usually 15 times greater than the volume at the CJ point) [5].

Up to now the program was tested on a series of explosives having different composition and different densities [1,5,6,7,8]. Generally, it was found out that a satisfactory agreement exists

between the calculated and experimental values of the detonation velocity and pressure. However, it is found that the calculated values of the detonation parametsrs are strongly affected by the values of constants used in the BKW equation of state [7,8,9]. I the previous paper [8] the set of constants was recalibrated taking into account an overall agreement, i.e. agreement between calculated and experimentally obtained values of the detonation velocity, pressure, temperature, heat, and composition of detonation products. The result of such recalibration was the set of constants named BKWN set: $\beta = 0.176$; $\kappa = 14.71$; $\alpha = 0.50$ and $\theta = 6620$ [8].

Results and Discussion

Several standard high explosives, for which experimental data for detonation parameters have been reported in literature, were chosen for the study in this paper. The detonation parameters were calculated for these explosives applying BKWN set of the constants in BKW EOS. The results of calculation are given in Table 1, along with the values obtained experimentally.

Two values of the detonation heat are given in Table 1. The value assigned as Q_{CJ} is the detonation heat at the CJ point, while the value assigned as Q_{1800} is the heat that corresponds to the state on the expansion isentrope at temperature 1800 K. This temperature is usually taken as the temperature at which all chemical reactions in the detonation products stop and composition of the detonation products freezes (freeze point). The value of detonation heat at the freeze point is comparable with calorimetricaly determined detonation heat [6].

The results given in Table 1 are analysed in more details in order to judge the applicability of computer program EXPLO5 for calculation of the main detonation parameters.

Detonation Velocity and Pressure. The comparison between calculated and experimental values of detonation velocity for explosives given in Table 1, is presented graphically in Fig. 1a. One can note that EXPLO5 gives consistently slightly greater values of detonation velocity, however, it should be stressed that the difference between the calculated and experimental values of detonation velocity is less than 5% in all cases.

The calculated values of detonation pressures for explosives given in Table 1 differ up to about 10 % from those obtained experimentally (Fig. 1b).

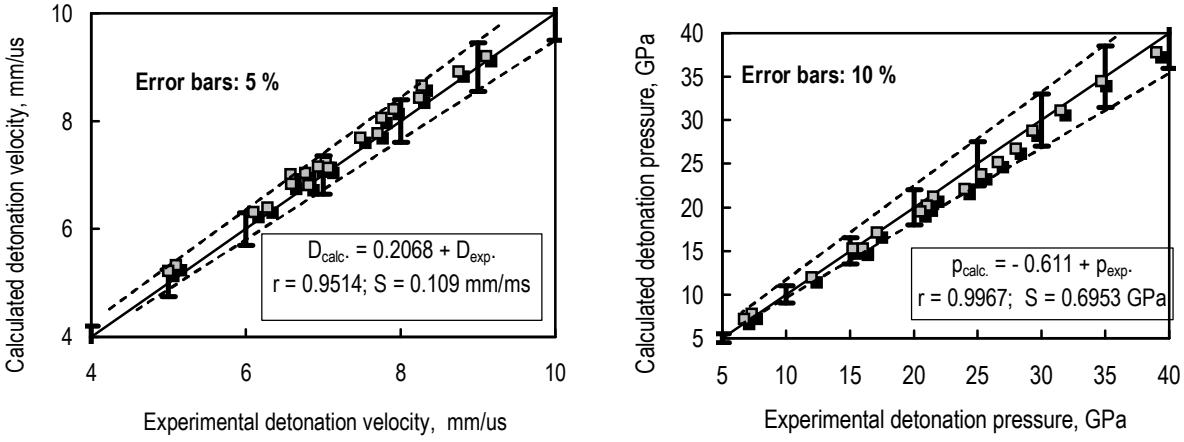

Fig. 1. Comparison of experimental and calculated values of detonation velocity (a) and detonation pressure (b)

Detonation Temperature and Detonation Heat. The values of detonation temperature at the CJ point calculated by EXPLO5 are compared to the values determined experimentally by Y. Kato [10]. The results of comparison are presented in Fig. 2. It is visible from Fig. 2 that a satisfactory agreement exist between calculated and experimentally obtained values of detonation temperature – the difference is up to about 5%. It was shown in the paper [8] that the values of detonation

temperature calculated applying the BKWR set of constants are lower than those obtained experimentally for about 550 K (mean difference), i.e. nearly 20%, while the worst agreement was obtained if the RDX/TNT set of constants is used: the calculated values of detonation temperature are lower than those obtained experimentally for about 1074 K (mean difference), i.e. nearly 40%.

Table 1. Comparison of calculated and experimental values of some detonation parameters

Explosive	Density, [g/cm^3]		D, [mm/μs]	P, [GPa]	T, [K]	Q_{CJ}, [kJ/kg]	Q_{1800}, [kJ/kg]
HMX	1.89	Experim.	9.11	39.0	–	–	5719
		EXPLO5	9.21	37.8	4286	6030	5818
	1.60	Experim.	7.91	28.0	4300	–	–
		EXPLO5	8.22	26.7	4357	5809	5533
	1.20	Experim.	6.58	16.0	–	–	5116
		EXPLO5	7.01	15.1	4264	5194	5284
HNS	1.65	Experim.	7.03	21.5	–	–	4432
		EXPLO5	7.23	21.2	4079	5239	4794
	1.00	Experim.	5.10	7.3	–	–	4550
		EXPLO5	5.33	7.8	3885	4341	4070
PETN	1.76	Experim.	8.27	31.5	–	–	5739
		EXPLO5	8.66	31.1	4349	5889	5932
	1.60	Experim.	7.75	26.6	4400	–	–
		EXPLO5	8.05	25.2	4425	5883	5935
	1.50	Experim.	7.48	24.0	–	–	5824
		EXPLO5	7.69	22.1	4468	5876	5937
	1.26	Experim.	6.59	16.0	–	–	5817
		EXPLO5	6.83	15.3	4553	5850	5944
NM	1.13	Experim.	6.28	12.0	3430	–	4482
		EXPLO5	6.40	12.0	3583	5137	4650
TNT	1.64	Experim.	6.95	21.0	–	–	–
		EXPLO5	7.15	20.2	3744	5087	4710
	1.63	Experim.	7.07	20.5	–	–	4270
		EXPLO5	7.13	19.5	3718	5074	4670
	1.53	Experim.	6.81	17.1	–	–	4382
		EXPLO5	6.81	17.1	3719	4982	4538
	1.00	Experim.	5.00	6.7	3400	–	–
		EXPLO5	5.22	7.2	3550	4322	3998
RDX	1.80	Experim.	8.75	34.7	–	–	5610
		EXPLO5	8.92	34.5	4354	6033	5810
	1.66	Experim.	8.24	29.3	4320	–	–
		EXPLO5	8.44	28.8	4376	5922	5655
	1.20	Experim.	6.77	15.2	4610	–	–
		EXPLO5	7.04	15.3	4314	5256	5346
	1.00	Experim.	6.10	–	4600	–	–
		EXPLO5	6.31	10.7	4389	5255	5252
NGl	1.60	Experim.	7.70	25.3	4260	–	–
		EXPLO5	7.77	23.8	4596	6073	6312

Notes: - Values of detonation velocity and pressure are according to M. Hobbs abd M. Bear (Ref. [9])
- Values of detonation temperature are according to Y. Kato (Ref. [10]
- Values of detonation heat are recalculated from D. Ornellas (Ref. [11]) and I. Akst (Ref. [12]), taking water to be gaseous.

The heat of detonation and composition of detonation products cannot be measured in a simple way – in a calorimeter. The values of the heat of detonation determined calorimetricaly by Ornellas

[11] are not values at the CJ point, but values over the freeze-out region on the expansion isentrope. The temperature of 1800 K is usually taken as the freeze point, i.e. point on the expansion isentrope at which all chemical reactions stop and composition of detonation products freezes. EXPLO5 is designed in the way that enables to halt all chemical reactions and freeze the products composition at 1800 K (or some other selected temperature). The heat of detonation corresponding to this temperature, assigned as Q_{1800}, should be thus comparable with Ornellas' calorimetricaly determined heat of detonation.

The results of comparison of calorimetricaly determined detonation heats and calculated detonation heats at the chemical equilibrium freeze point are presented graphically in Fig. 2. It follows from Fig. 2 that EXPLO5 gives the heats of detonation that differ up to 10% from the heats determined calorimetricaly. Other sets of constants in BKW EOS give the larger errors [8,9].

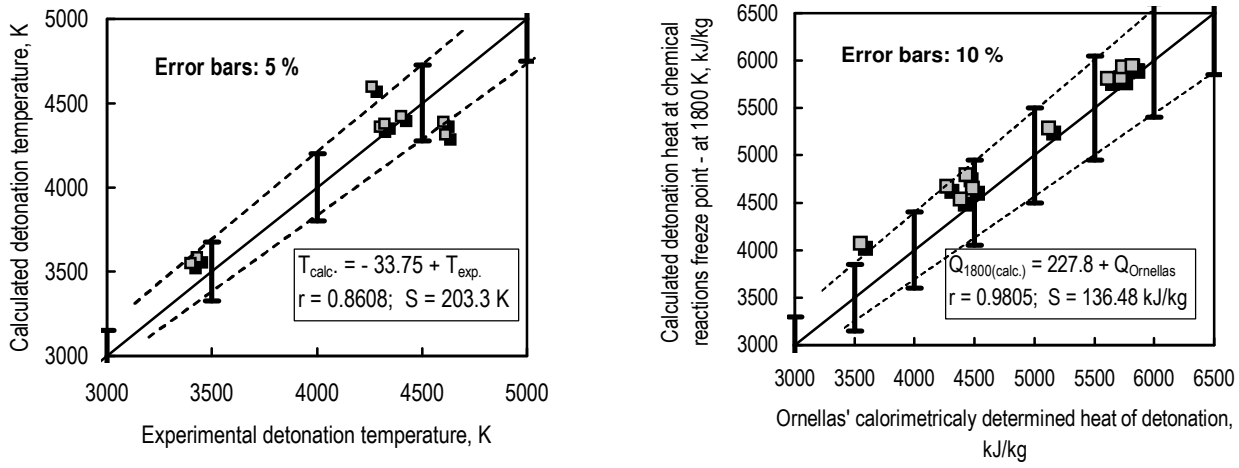

Fig. 2. Comparison of experimental and calculated values of detonation temperature (a) and detonation heat (b)

Detonation Energy. The detonation energy (E_0), as a very important detonation parameter of an explosive that can be related with the cylinder wall velocity, can be evaluated from the results of thermochemical computer codes [6,12,13]. In the previous paper [5] it was shown that the detonation energy could be derived from EXPLO5 results in two ways:

- directly from the detonation heat, i.e. by equating detonation energy with the heat of detonation at the CJ point ($E_0 = Q_{CJ}$)
- evaluation of detonation energy applying JWL model, i.e. describing the expansion of detonation products by the JWL equation of state and integrating pressure-volume data to derive energy on the isentrope.

The detonation energies for several high explosives for which cylinder test evaluated detonation energies and JWL coefficients have been reported in literature were calculated by EXPLO5 in accordance to the procedure described in more details in papers [5,13]. The results of calculations are given in Table 2.

It is important to note that in this paper the fitting of pressure-volume data on the expansion isentrope in order to derive the detonation energy, is performed without any constraints – that means that the JWL coefficients are allowed to have any value. The JWL coefficients obtained in this way from EXPLO5 results and the detonation energies calculated from the JWL coefficients derived, are shown in Table 2, along with the values reported in literature [13, 14] derived from cylinder test data.

Table 2. The JWL coefficients and detonation energies determined in this work and derived from cylinder test data

Explosive	ρ_0, [g/cm^3]		A, [Mbar]	B, [Mbar]	C, [Mbar]	R_1	R_2	ω	E_0, [kJ/cm^3]	Q_{CJ}, [kJ/cm^3]	Q_{1800}, [kJ/cm^3]
HMX	1.894	(1)	23.93191	1.317629	0.092322	7.08695	3.3236	1.2669	-10.39	-11.43	-11.05
		(2)	8.580805	0.0754653	0.0078127	4.306	0.80	0.30	-11.00		
HMX	1.188	(1)	4.691025	0.1812784	0.0333264	5.95321	2.2974	0.79939	-5.79	-6.35	-6.30
		(2)	2.182000	0.0495943	0.0197717	4.379	1.10	0.55	-6.40		
HNS	1.655	(1)	10.97389	0.555288	0.0459076	6.66001	2.9264	0.93778	-6.94	-8.67	-7.94
		(2)	4.237580	0.0313147	0.0170416	4.332	1.00	0.40	-7.50		
HNS	1.001	(1)	2.934041	0.184646	0.0218977	7.04109	2.9578	0.77159	-3.55	-4.36	-4.08
		(2)	1.388149	0.0277983	0.0069414	4.657	1.00	0.35	-3.60		
PETN	1.763	(1)	28.38018	1.159409	0.0801459	7.69091	3.3572	1.14897	-9.52	-10.38	-10.45
		(2)	10.32158	0.9057014	0.0372735	6.000	2.60	0.57	-10.80		
PETN	1.503	(1)	15.89802	0.683061	0.0589224	7.54385	3.1890	0.98535	-7.85	-8.83	-8.92
		(2)	3.510723	0.0570555	0.0121624	4.075	0.90	0.35	-8.50		
PETN	1.263	(1)	8.544155	0.3890708	0.0425993	7.35651	3.0123	0.84318	-6.41	-7.39	-7.50
		(2)	2.281744	0.0510458	0.0141201	4.240	1.05	0.35	-7.20		
NM	1.13	(1)	5.714129	0.2424576	0.0189663	6.77279	2.1275	0.76704	-4.47	-5.81	-5.08
		(2)	2.977799	0.0595492	0.0110800	5.026	1.10	0.49	-4.95		
TNT	1.632	(1)	12.21087	0.5314439	0.0445601	6.84575	2.9630	0.94127	-6.61	-8.29	-7.66
		(2)	5.244089	0.0490005	0.0062613	4.579	0.85	0.23	-7.10		
CompB	1.717	(1)	15.82063	0.8016194	0.0672026	6.92275	3.1288	1.11675	-8.42	-9.74	-9.25
		(2)	4.96376	0.03944	0.01288	4.06244	0.9485	0.35	-8.50		
Cyclotol	1.754	(1)	17.72528	0.9213422	0.0735505	6.98693	3.1784	1.15180	-8.97	-10.18	-9.72
		(3)	5.60038	0.05131	0.01361	4.12004	0.9951	0.35	-9.20		

Legend:

(1) - derived from EXPLO5 results using BKWN set of constants in BKW EOS

(2) - derived from cylinder test (values taken from Souers and Kury) [13]

(3) - derived from cylinder test (values taken from Hornberg) [14]

A, B, C, R_1, R_2 and ω are coeficients in JWL EOS ($p = A\exp(-R_1 v) + B\exp(-R_2 v) + Cv^{-(1+\varpi)}$)

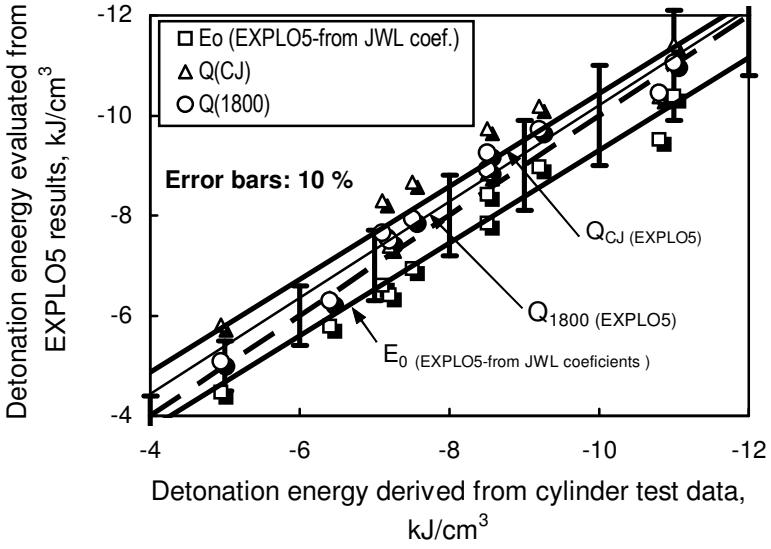

Fig. 3. Detonation heats and energies derived from EXPLO5 results *vs*. detonation energies evaluated from cylinder test data

From graphic presentation given in Fig. 3 it is clear that the detonation energies derived from EXPLO5 results in accordance with the JWL model, differ up to 10% in respect to the energies derived experimentally from the cylinder test results. Also, it is visible that the values of Q_{CJ} are greater up to 15% than detonation energies, while at the same time the values of Q_{1800} are closer to the values of detonation energies – difference is less than 10%.

It can be noted from Table 2 that the JWL's coefficients derived from EXPLO5 results by nonlinear fitting procedure, deviate considerably compared to those derived from cylinder test data and given in [13, 14]. This is primarily consequence of different approach in the evaluation of the JWL coefficients – are there any constrains or not. Although the obvious way to generate the JWL coefficients is from the pressure-volume-energy results of computer codes, in this work they are evaluated from the pressure-volume space only. This approach has the following advantages: detonation energy is evaluated truly from EXPLO5 results (no experimentally determined parameters are required as input parameters for fitting). On the other hand, the values of detonation energies obtained in this way are in acceptable agreement with values derived from cylinder test experimental data.

Conclusions

The results of this work have shown that EXPLO5 computer program can be used for the calculation of detonation velocity, pressure, temperature, heat, and energy with the error less than 10% in respect to the experimentally obtained values. It was also shown that an own set of constants in BKW EOS, named BKWN set, gives the best overall agreement, although other sets of constants (RDX/TNT and BKWR) can give better results for the detonation velocity and pressure, but very poor results for the detonation temperate and heat .

It was shown that it is possible to derive detonation energy, from detonation heat or from the expansion isentrope of detonation products, without any constrains and without any experimental data as input parameters.

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