Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 77 (3) 371–380 (2012)
JSCS–4275
UDC 662.21:662.215.2:519.87
Original scientific paper

Development of a new model for the calculation of the detonation parameters of high explosives

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(Received 6 December 2010)

Abstract: A simple semi-empirical model for the calculation of the detonation pressure and velocity for CHNO explosives has been developed, which is based on experimental values of the detonation parameters. Model uses the Avakyan method for the determination of the chemical composition of the detonation products, and is applicable over a wide range of densities. Compared with the well-known Kamlet method and the numerical model of detonation based on the Becker–Kistiakowsky–Wilson Equation of state (BKW EOS), the calculated values from the proposed model have significantly better accuracy.

Keywords: detonation modeling; detonation velocity; detonation pressure; CHNO high explosives.

INTRODUCTION

The possibility of accurate prediction of their detonation characteristics significantly shortens the process of the development of new explosives, consequently lowering the development costs.

Two approaches are usually used in this issue. The first is based on numerical modeling of detonation and the second on much simpler empirical and semi-empirical models.

Laboratories in developed countries, especially in the USA, developed the first computer programs for numerical modeling of detonation more than 40 years ago. In the last years, they have work on improvements of the numerical models for non-stationary detonation.

Mader and his co-workers from the Los Alamos National Laboratory, using the Becker-Kistiakowsky-Wilson Equation of state (BKW EOS), developed the program STRETCH BKW for the calculation of detonation parameters in 1961.[1,2] For that time, the program had a high rate of calculations with acceptably accurate results. The program used only one set of parameters of the BKW Equation of state for all explosives.

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doi: 10.2298/JSC101206163J

Mader also developed computer program Fortran BKW in 1967, which has been used in research institutions in many countries. Up to now, the program was modified several times to be compatible with modern computer software.[1-4]

Other programs using the BKW EOS, such as Arpage and La Mineur, were also developed.[4] The program Tiger used the Jacobs–Cowperthwaite–Zwisler Equation of state (JCZ EOS).[5]

The numerical models are not always suitable for engineering purposes, mainly because of their complexity. Therefore, many different empirical and semi-empirical methods of calculation have been developed, which are much simpler for use. The most famous is the Kamlet method, which gives acceptably accurate results for CHNO high explosives with an initial density above 1000 kg m^{-3}.[6]

A new simple semi-empirical method for the prediction of the detonation parameters of CHNO high explosives is presented in this work. The differences between experimental values and calculation results obtained with this new method are significantly smaller when compared to the numerical model and the Kamlet method.

THEORETICAL BASICS OF THE METHOD

The relations between the detonation pressure p (in the Chapman-Jouguet or C-J point), detonation velocity D, initial density of explosive ρ_0 and heat of detonation Q are known from the hydrodynamic theory of detonation:[7]

$$D = \sqrt{2(\gamma^2 - 1)Q} \tag{1}$$

$$p = \frac{1}{\gamma + 1}\rho_0 D^2 \tag{2}$$

where γ is the polytropic exponent.

Combining Eqs. (1) and (2), it follows:

$$p = 2(\gamma - 1)\rho_0 Q \tag{3}$$

Considering the fact that the experimental values of the detonation parameters are proportional to the initial density of the explosive[1,2] and that, based on the EOS of gases, the pressure is proportional to the number of moles of gaseous detonation products, n, Eq. (3) can be written in the following general form:

$$p = A\rho_0^2 nQ \tag{4}$$

where A is an empirical constant.

Numerous experiments showed that the dependence of the detonation velocity on the initial density is linear for all explosive charges above a critical diameter, which can be represented as:[7]

$$D = D_1 + M(\rho - \rho_1) \tag{5}$$

where D_1 is the detonation velocity for an initial density ρ_1 and M is an empirical constant.

Combination of the Eqs. (4) and (2) and considering Eq. (5) the following general equation for calculation of detonation velocity can be written as:

$$D = B + C\rho_0\sqrt{nQ} \quad (6)$$

where B and C are empirical constants.

The empirical constants in Eqs. (4) and (6) can be obtained using regression analysis of the experimental data for the dependence of detonation pressure and velocity on the initial density of the explosive.

The number of moles of gaseous detonation products, n, can be easily calculated using the Avakyan method.[7] According to Avakyan's experimental data, the coefficient of realization (K) can be calculated from the oxygen coefficient (K_k) using the following equation:

$$K = 0.32\ K_k^{0.24} \quad (7)$$

in which the oxygen coefficient should be expressed in percents.

If the presence of ammoniac in the detonation products is neglected, the summary chemical reaction of detonation can be written as:

$$C_xH_yN_zO_u \rightarrow n_1H_2O + n_2H_2 + n_3CO_2 + n_4CO + n_5O_2 + n_6N_2 + n_7C \quad (8)$$

The calculation of the chemical composition of the detonation products is based on the assumption that the coefficient of realization K determines the degree of hydrogen oxidation and formation of water. In other words, it is assumed that from $y/2$ (maximal possible value) moles of hydrogen, $Ky/2$ moles of water are formed during the explosion, while $(1 - K)y/2$ moles remain as H_2. According to this:

$$n_1 = Ky/2,$$
$$n_2 = (1 - K)y/2$$

The number of moles of nitrogen can be calculated as:

$$n_6 = z/2$$

For the remaining detonation products, it is necessary to solve a system of equations, representing the mass and energy balance, considering the ratio of oxygen, carbon and hydrogen in the composition of the explosive. Depending on this ratio, three characteristic cases should be considered.

Case 1. $K_k > 100$ %: It is assumed that there is no formation of free carbon in the detonation products, *i.e.*, $n_7 = 0$. The following equations are used for the calculation of n_3–n_5:

$$n_3 = (1.4K - 0.4)x$$
$$n_4 = x - n_3 = 1.4x(1 - K)$$
$$n_5 = (x - 2n_3 - n_4 - n_1)/2$$

Case 2. $K_k < 100$ %: It is assumed that there is no formation of free oxygen in the detonation products, *i.e.* $n_5 = 0$. The remaining detonation products are determined using the following equations:

$$n_3 = 1.16u\ (K - 0.568) - 0.5n_1$$
$$n_4 = u - (2n_3 + n_1) = u\ (1 - 2.32\ (K - 0.568))$$
$$n_7 = x - (n_3 + n_4)$$

Case 3. $K_k < 100$ % and $u > (x + y/2)$: The following equations are used:

$$n_3 = 0.7\ (u - y/2)K - 0.4x$$
$$n_4 = 1.4x - 0.7\ (u - y/2)K$$
$$n_5 = 0 \text{ and } n_7 = 0$$

In the next step, the total heat of formation for the determined detonation products is calculated. The heat of explosion is then determined using the Hess Law as:

$$Q = \sum_{i=1}^{n} \Delta U^0_{f_{i\text{prod}}} - \sum_{j=1}^{m} \Delta U^0_{f_{i\text{EM}}} \quad (9)$$

where i =1,…, n is the index of a particular detonation product, while j = 1,…, m is the index number of the individual components of the explosion.

The heat of formation data for components of the explosion and the detonation products can be found in thermochemical tables.[2,4,7,10]

It should be noted that the Avakyan method predicts the chemical composition of the detonation products after expansion and cooling.

APPLICATION AND EVALUATION OF THE MODEL

The proposed model was applied for the calculation of the detonation parameters of 72 explosive compositions (25 different explosives with various initial densities), the detonation pressures and velocities of which had previously been experimentally determined (Table I). The amounts of the individual detonation products were first calculated using the Avakyan method.

The empirical constants in Eqs. (4) and (6) were determined using the regression analysis of the results (Figs. 1 and 2):

$$\rho = 0.00048\rho_0^2 nQ \quad (10)$$

$$D = 2264.1 + 7.7072\rho_0\sqrt{nQ} \quad (11)$$

In the previous equations, the initial density, ρ_0, is expressed in g cm^{-3}, the total quantity of gaseous detonation products, n, is in mol kg^{-1} and the heat of explosion, Q, is in kJ kg^{-1}. The calculated detonation pressure p is in kbar, and the detonation velocity D is in m s^{-1}.

Comparisons of the calculated detonation parameters with their differences from the appropriate experimental values are presented in Tables I–III. The high value of the correlation coefficient (R^2 > 0.98) for the 74 considered explosive compositions shows that the proposed model could be successfully employed in the theoretical determination of the detonation parameters.

The average differences between the calculated detonation parameters and the experimental values are presented in Table IV. Compared with the BKW EOS or the Kamlet method, the proposed model gives significantly more precise calculation results. In addition, the calculation results have a similar precision to those obtained using the numerical model XWizard.[11] The proposed model is also applicable over a much wider range of initial densities, which is not possible with the other models. The precision of calculation results for explosives with high values of initial density are also acceptable, as presented in Tables I–III.

The obtained differences between the calculated results and the experimental values are within the expected experimental error. It should be mentioned that ex-

TABLE I. Comparison of differently determined detonation parameters for explosives (TNT, 2,4,6-trinitrotoluene; RDX, 1,3,5-trinitro-2,4,6--triazacyclohexane; HMX, 1,3,5,7-tetranitro-2,4,6,8-tetraazacyclooctane; PETN, pentaerythritol tetranitrate; Tetryle7, *N*-methyl-*N*-2,4,6-tetranitroaniline; NM, nitromethane; NGL, nitroglycerine; HNS, 2,2',4,4',6,6'-hexanitrodiphenylethylene (hexanitrostilbene); DATB, 1,3-diamino-2,4,6-trinitrobenzene)

Explosive	ρ_0 g cm^{-3}	Experiment		BKW		Kamlet		Model		Difference, %					
										BKW		Kamlet		Model	
		p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}
RDX2,7	0.70	59.9	4989	60	5222	51.7	5026	51.2	4781	0.2	4.7	−13.7	0.7	−14.5	−4.2
	1.00	108	6030	104	6044	105.6	6052	104.5	5860	−3.7	0.2	−2.2	0.4	−3.2	−2.8
	1.29	166.2	7036	168	6922	175.7	7044	173.9	6903	1.1	−1.6	5.7	0.1	4.6	−1.9
	1.46	209.8	7626	215	7491	225.1	7626	222.7	7514	2.5	−1.8	7.3	0.0	6.2	−1.5
	1.59	259	8077	263	7962	267	8071	264.2	7982	1.5	−1.4	3.1	−0.1	2.0	−1.2
	1.72	310	8528	311	8467	312.4	8515	309.1	8449	0.3	−0.7	0.8	−0.2	−0.3	−0.9
	1.80	347	8754	339	8795	342.2	8789	338.6	8737	−2.3	0.5	−1.4	0.4	−2.4	−0.2
HMX2,10	1.77	323	8500	339.8	8708	327.8	8646	314.1	8499	5.2	2.4	1.5	1.7	−2.7	0.0
	1.90	393	9100	391	9288	380.5	9123	362	8957	−0.5	2.1	−3.2	0.3	−7.9	−1.6
TNT2,7	0.80	36.4	4340	55	4806	48.6	4551	45.39	4634	51.1	10.7	33.5	4.9	24.7	6.8
	1.00	62.5	5100	81	5319	75.9	5131	70.92	5227	29.6	4.3	21.4	0.6	13.5	2.5
	1.36	122.2	6200	146	6310	140.4	6175	131.2	6293	19.5	1.8	14.9	−0.4	7.3	1.5
	1.45	142	6500	166	6576	159.6	6436	149.1	6560	16.9	1.2	12.4	−1.0	5.0	0.9
	1.59	176.5	6940	198	7010	191.9	6842	179.3	6975	12.2	1.0	8.7	−1.4	1.6	0.5
	1.64	190	6950	215	7169	204.1	6987	190.8	7123	13.2	3.2	7.4	0.5	0.4	2.5
PETN2	0.25	7	2830	11	3414	6.6	3493	6.261	3144	57.1	20.6	−5.7	23.4	−10.6	11.1
	0.50	24	3800	30	4692	26.5	4349	25.04	4025	25.0	23.5	10.4	14.4	4.3	5.9
	1.00	97	6025	107	6026	106	6063	100.2	5785	10.3	0.0	9.3	0.6	3.3	−4.0
	1.67	300	7980	279	8050	295.5	8358	279.4	8144	−7.0	0.9	−1.5	4.7	−6.9	2.1
	1.77	335	8300	318	8424	332	8701	313.8	8496	−5.1	1.5	−0.9	4.8	−6.3	2.4
Tetryle7	0.90	64.6	5360	76	5316	71	5203	72.2	5253	17.6	−0.8	9.9	−2.9	11.8	−2.0
	1.36	140	6680	160	6616	162.2	6637	164.9	6781	14.3	−1.0	15.9	−0.6	17.8	1.5
	1.70	245	7560	253	7750	247.5	7634	257.6	7910	3.3	2.5	1.0	1.0	5.1	4.6
NM2	1.13	125	6523	138	6590	130.2	6383	118.8	6099	10.4	1.0	4.2	−2.1	−4.9	−6.5
NGL2	1.59	246	7580	245	7641	281.6	8289	232.3	7625	−0.4	0.8	14.5	9.4	−5.6	0.6
HNS11	1.70	210	7000	233.4	7255	219.3	7159	196.8	7199	11.1	3.6	4.4	2.3	−6.3	2.8
DATB10	1.79	259	7520	239	7637	253.3	7574	237.9	7690	−7.7	1.6	−2.2	0.7	−8.2	2.3
Average difference of the results, %										12.2	3.5	8.0	3.0	6.9	2.8

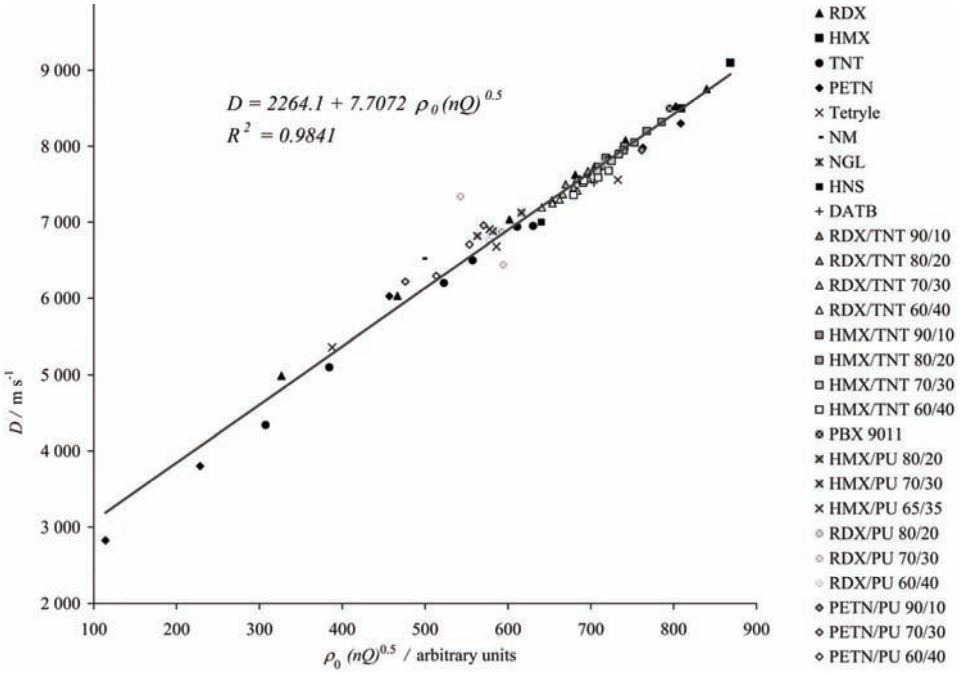

Fig. 1. Calculated and experimental values of the detonation velocity.

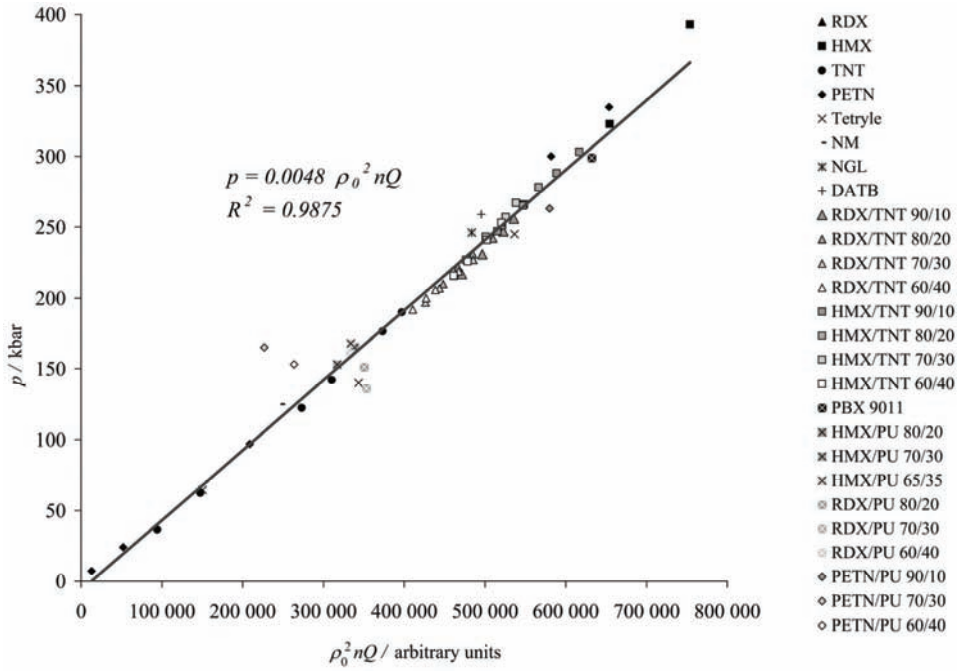

Fig. 2. Calculated and experimental values of the detonation pressure.

TABLE II. Comparison of differently determined detonation parameters for explosive mixtures with TNT

Explosive	ρ_0 g cm^{-3}	Experiment		BKW		Kamlet		Model		Difference, % BKW		Kamlet		Model	
		p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}
RDX/TNT 90/10[9]	1.51	217	7570	230	7599	234.1	7687	226.3	7556	6.0	0.4	7.9	1.5	4.3	–0.2
	1.55	231	7740	240	7744	245.5	7805	238.4	7696	3.9	0.1	6.3	0.8	3.2	–0.6
	1.59	247	7840	251	7892	243.6	7709	250.9	7836	1.6	0.7	–1.4	–1.7	1.6	0.0
	1.61	256	7910	264	7967	242.3	7657	257.3	7906	3.1	0.7	–5.4	–3.2	0.5	0.0
RDX/TNT 80/20[9]	1.50	210	7500	223	7494	223.7	7532	215.3	7426	6.2	–0.1	6.5	0.4	2.5	–1.0
	1.53	222	7570	231	7601	232.7	7632	224	7529	4.1	0.4	4.8	0.8	0.9	–0.5
	1.56	231	7675	238	7709	238	7709	232.9	7632	3.0	0.4	3.0	0.4	0.8	–0.6
	1.60	242	7745	256	7858	254.5	7864	244.9	7770	5.8	1.5	5.2	1.5	1.2	0.3
RDX/TNT 70/30[9]	1.49	197	7290	210	7386	213.9	7382	204.7	7298	6.6	1.3	8.6	1.3	3.9	0.1
	1.52	207	7370	224	7492	222.6	7480	213.1	7399	8.2	1.7	7.5	1.5	2.9	0.4
	1.55	216	7460	231	7600	231.5	7578	221.6	7500	6.9	1.9	7.2	1.6	2.6	0.5
	1.59	227	7580	242	7747	243.6	7709	233.1	7635	6.6	2.2	7.3	1.7	2.7	0.7
RDX/TNT 60/40[9]	1.49	192	7195	206	7312	207.5	7271	197.1	7203	7.3	1.6	8.1	1.1	2.7	0.1
	1.52	200	7250	213	7420	216	7368	205.1	7302	6.5	2.3	8.0	1.6	2.6	0.7
	1.54	206	7300	224	7490	221.7	7432	210.6	7369	8.7	2.6	7.6	1.8	2.2	0.9
	1.59	219	7415	237	7675	236.3	7593	224.5	7535	8.2	3.5	7.9	2.4	2.5	1.6
HMX/TNT 90/10[9]	1.60	247	7850	263	7967	262.4	7984	247.5	7799	6.5	1.5	6.2	1.7	0.2	–0.7
	1.65	266	8000	278	8157	279	8153	263.2	7972	4.5	2.0	4.9	1.9	–1.0	–0.4
	1.71	288	8200	305	8390	299.7	8355	282.7	8179	5.9	2.3	4.1	1.9	–1.8	–0.3
	1.75	303	8320	318	8550	313.9	8490	296.1	8317	5.0	2.8	3.6	2.0	–2.3	0.0
HMX/TNT 80/20[9]	1.61	242	7730	261	7928	257.3	7891	241.2	7727	7.9	2.6	6.3	2.1	–0.4	0.0
	1.64	251	7820	270	8042	267	7991	250.2	7829	7.6	2.8	6.4	2.2	–0.3	0.1
	1.68	265	7950	282	8197	280.2	8123	262.6	7964	6.4	3.1	5.7	2.2	–0.9	0.2
	1.71	278	8050	299	8314	290.3	8223	272	8066	7.6	3.3	4.4	2.1	–2.1	0.2
HMX/TNT 70/30[9]	1.60	227	7520	247	7815	246.5	7738	228.9	7587	8.8	3.9	8.6	2.9	0.9	0.9
	1.64	243	7680	265	7965	258.9	7869	240.5	7720	9.1	3.7	6.5	2.5	–1.0	0.5
	1.68	257	7810	277	8119	271.7	7999	252.4	7853	7.8	4.0	5.7	2.4	–1.8	0.6
	1.70	267	7900	283	8197	278.2	8065	258.5	7920	6.0	3.8	4.2	2.1	–3.2	0.2
HMX/TNT 60/40[9]	1.60	216	7360	242	7737	239	7621	221.4	7499	12.0	5.1	10.6	3.5	2.5	1.9
	1.63	226	7550	257	7850	248.1	7717	229.8	7597	13.7	4.0	9.8	2.2	1.7	0.6
	1.67	241	7590	268	8000	260.4	7846	241.2	7728	11.2	5.4	8.0	3.4	0.1	1.8
	1.70	253	7680	278	8118	269.8	7942	249.9	7826	9.9	5.7	6.6	3.4	–1.2	1.9
Average difference of the results, %										7.0	2.4	6.4	1.9	1.8	0.6

TABLE III. Comparison of differently determined detonation parameters for explosive mixtures with TNT (PBX-9011, plastic-bonded high explosive with 90 % HMX and 10 % polymer binder (polyurethane, Estane 5701 F-1); PU, polyurethane binder)

Explosive	ρ_0 g cm^{-3}	Experiment		BKW		Kamlet		Model		Difference, %					
										BKW		Kamlet		Model	
		p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	p kbar	D m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}
PBX-9011[10]	1.77	299	8500	331	7700	301.9	8297	303.4	8392	10.7	−9.4	1.0	−2.4	1.5	−1.3
HMX/PU 80/20[4]	1.35	165	6880	175	7026	165	6712	162.4	6748	6.1	2.1	0.0	−2.4	−1.5	−1.9
	1.43	188	7126	193	7335	185.1	6966	182.3	7013	2.7	2.9	−1.5	−2.2	−3.0	−1.6
HMX/PU 70/30[4]	1.33	153	6818	164	6920	149.4	6423	152.2	6604	7.2	1.5	−2.4	−5.8	−0.5	−3.1
HMX/PU 65/35[4]	1.39	168	6906	182	6831	156.4	6466	160.3	6718	8.3	−1.1	−6.9	−6.4	−4.6	−2.7
RDX/PU 80/20[4]	1.30	151	6870	157	6802	154.2	6579	168.3	6827	4.0	−1.0	2.1	−4.2	11.4	−0.6
	1.57	234	7778	242	7870	242	7870	245.4	7775	3.4	1.2	3.4	1.2	4.9	0.0
RDX/PU 70/30[4]	1.26	136	6441	143	6612	131.5	6146	169.6	6845	5.1	2.7	−3.3	−4.6	24.7	6.3
	1.38	167	7339	173	7090	157.7	6510	141.4	6447	3.6	−3.4	−5.6	−11.3	−15.3	−12.2
RDX/PU 60/40[4]	1.36	161	6765	172	7201	139.5	6156	159.9	6712	6.8	6.4	−13.4	−9.0	−0.7	−0.8
PETN/PU 90/10[4]	1.65	263	7950	269	8027	268.5	7997	278.4	8134	2.3	1.0	2.1	0.6	5.9	2.3
PETN/PU 70/30[4]	1.16	115	6218	119	6110	117.4	5999	108.8	5934	3.5	−1.7	2.1	−3.5	−5.4	−4.6
	1.39	165	6957	174	6870	168.6	6714	156.3	6662	5.5	−1.3	2.2	−3.5	−5.3	−4.2
PETN/PU 60/40[4]	1.28	129	6294	140	6428	128.1	6032	126.6	6221	8.5	2.1	−0.7	−4.2	−1.9	−1.2
	1.38	153	6708	164	6787	148.9	6326	147.1	6531	7.2	1.2	−2.7	−5.7	−3.9	−2.6
Average difference of the results, %										5.7	2.6	3.3	4.5	6.0	3.0

TABLE IV. Comparison of the average differences of the calculated detonation parameters

Type of explosivecomposition	Number of considered compositions	Difference, %					
		BKW		Kamlet		Model	
		Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}	Δp kbar	ΔD m·s^{-1}
Explosives	27	12.2	3.5	8.0	3.0	6.9	2.8
Explosive mixtures with TNT	32	7.0	2.4	6.4	1.9	1.8	0.6
Plastic-bonded explosives	15	5.7	2.6	3.3	4.5	6.0	3.0
Average difference of results, %		8.6	2.9	6.4	2.8	4.5	1.9

perimental values of detonation pressure and velocity in literature are quite different, mainly due to the low accuracy of the experimental methods. While modern experimental methods can determine detonation velocities with an accuracy below 1 %, the experimental values of the detonation pressure are expected to have an error above 10 %.[7]

CONCLUSIONS

A new, simple semi-empirical model for the calculation detonation pressure and velocity of CHNO high explosives is presented in this paper. The model is based on the theoretical model of an ideal detonation. The Avakyan method was used for the determination of the chemical composition of the detonation products. A good correlation between the calculated and experimental detonation parameters over a wide range of initial densities was achieved, and the results are within the degree of experimental error. In addition, the proposed model can be used for the calculation of the detonation pressure and velocity for explosives with the maximum initial density. The average difference of the calculation results was approximately 50 % smaller than the results obtained from a numerical model and by the Kamlet method.

ИЗВОД

РАЗВОЈ НОВОГ МОДЕЛА ЗА ПРОРАЧУН ДЕТОНАЦИОНИХ ПАРАМЕТАРА БРИЗАНТНИХ ЕКСПЛОЗИВА

РАДУН ЈЕРЕМИЋ и ЈОВИЦА БОГДАНОВ

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У складу са теоријом идеалне детонације, а на основу експерименталних вредности детонационих параметара већег броја бризантних експлозива и различитих експлозивних састава, развијен је једноставан полуемпиријски модел за прорачун притиска и брзине детонације експлозива типа "CHNO". Модел је заснован на Авакјановој методи за прорачун састава гасовитих продуката детонације и применљив је у широком опсегу густина. Добијене вредности притиска и брзине детонације много мање одступају од експерименталних вредности у односу на познату Камлетову методу и нумерички модел заснован на БКW једначини стања.

(Примљено 6. децембра 2010)

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