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A Simple Method for Calculating the Detonation Pressure of Ideal and Non-Ideal Explosives Containing Aluminum and Ammonium Nitrate

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Abstract: A general and simple method has been developed for calculating the detonation pressure of different kinds of ideal and non-ideal explosives containing aluminum (Al) and ammonium nitrate (AN). The new model can be applied to CHNO and CHNOFCl explosives in pure form or as mixtures as well as non-ideal mixed explosives including Al and AN. It can also be used for different plastic bonded explosives (PBXs). There is no need for any prior knowledge about the measured or calculated properties of the explosive. The only data needed are the standard enthalpy of formation and the loading density of the desired explosive. The predicted detonation pressures were compared with other predictive methods and outputs of BKWS-EOS, in both full and partial equilibrium. Different statistical parameters as well as cross validation parameters showed that the new model is precise, accurate, well-defined, and robust for predicting the detonation pressures of CHNOFCl(Al/AN) energetic materials.

Keywords: detonation pressure, ideal explosive, non-ideal explosive, cross validation

1 Introduction

The search for new energetic materials with high performance, low sensitivity, and appropriate physical properties is a continuing challenge for the military and demolition industries. When a new energetic material is synthesized or designed, its detonation performance and its sensitivity to external stimuli should be determined. Due to the difficulty, danger, and cost of experiments, it is important

to have reliable predictive methods for the assessment of a number of different properties before synthesis and testing. Theoretical and semi-empirical methods help chemists to develop systematically and scientifically new energetic materials having complementary properties of stability, sensitivity and performance [1]. The detonation performance of explosives is mainly defined in terms of detonation pressure (*DP*), detonation velocity (*VOD*), and strength [1, 2]. Different predictive methods with domains of various degrees of complexity and applicability have been proposed for calculating performance parameters. Several thermochemical equilibrium codes such as Explo5 [3] have been developed. Also the method of Kamlet and Jacobs [4], which is a common and well-known technique, is established for the prediction of *DP* and *VOD* of CHNO explosives with initial densities greater than 1 g/cm^3. This method can also be used for halogenated explosives [5, 6].

Due to the physical separation of fuel and oxidizer in explosives containing aluminum (Al) and/or ammonium nitrate (AN), secondary reactions occur between detonation products as the chemical reaction zone spreads. So the behavior of Al and/or AN explosives cannot be described by steady-state detonation calculations [7, 8]. So in order to consider such non-ideal behaviors, computer codes may assume partial equilibrium, *i.e.* consumption of a fraction of Al/AN [9]. Modeling non-ideal behavior is very complicated as it requires incorporation of reaction kinetics into the fluid-flow equations (*e.g.* Wood and Kirkwood model). The outputs of such codes are the self-propagating detonation velocity and pressure as a function of explosive charge diameter. However, Zhang and Chang [10] adjusted the parameter k in the BKW-EOS to obtain *DP* and *VOD* for Al explosives. Some semi-empirical models have also been proposed for predicting the performance of ideal explosives and non-ideal explosives containing Al [11, 12] and AN [9] based on the partial consumption of Al and AN.

The purpose of this research was to complete previous studies by introducing a new model for calculating the detonation pressure of important classes of ideal and non-ideal energetic compounds at various loading densities. The new model, which is constructed on the basis of a new decomposition scheme, can be used both for pure explosives or energetic mixtures with the general formula of CHNO or CHNOFCl, as well as plastic bonded explosives (PBXs) and composite explosives containing Al or AN, *i.e.* CHNOFClAlAN energetic materials.

2 Materials and Methods

Finding the equilibrium composition of the detonation products has great importance in the study of the behavior of a new explosive. In previous studies,

this has been achieved by the free energy minimization technique [13] in thermochemical equilibrium codes. The moles of gaseous products per gram of explosive (α), the average molecular weight of gaseous products ($\overline{MW}_g$), and the heat of detonation (Q_d) can be obtained through the reaction scheme. Equation 1 shows the formula for calculating the values of Q_d:

$$Q_d = -\frac{\left[\sum_i \Delta_f H^\theta(\text{products})_i - \Delta_f H^\theta(\text{c})\right]}{\text{formula weight of explosive}} \tag{1}$$

where $\Delta_f H^\theta(\text{products})_i$ and $\Delta_f H^\theta(\text{c})$ are the standard enthalpies of formation of the i^{th} product and the condensed phase standard enthalpy of formation of the explosive, respectively.

In Ref. [9] predictions were reported of the *VOD* for different CHNOFClAlAN explosives on the basis of a new reaction scheme containing twelve detonation products, *i.e.* N_2, C (graphite), CO, CO_2, H_2O, H_2, O_2, HF, HCl, Al_2O_3(s), Al(s), and NH_4NO_3(s). The study of the values of α, $\overline{MW}_g$, and Q_d obtained from this reaction scheme showed that it can also be used for the reliable prediction of the detonation pressure. After a widespread search through the literature, experimental values of *DP* have been collected for 111 pure and mixed energetic materials with the general formula $C_aH_bN_cO_dF_eCl_fAl_g(NH_4NO_3)_h$. As each value of *DP* corresponds to a particular loading density (ρ_0), the dataset contains 288 data points. It should be noted that all the experimental data points and predicted values refer to an infinite charge diameter.

Quantitative structure property relationship (QSPR) methods are used for correlating physical or chemical properties with molecular structures [14, 15]. In Ref. [9], it was shown that several decomposition paths based on oxygen balance can be used to evaluate ρ_0, α, $\overline{MW}_g$, and Q_d. It possible to use suitable combinations of these parameters and statistical tools to derive correlations for estimating the detonation pressure of different kinds of ideal and non-ideal explosives containing Al and AN. Multiple linear regression (MLR), which is a QSPR modeling method, is a multivariate statistical tool used to derive mathematical correlations between properties and descriptors [14, 16-18]. The MLR method was used to build the desired correlation between ρ_0, α, $\overline{MW}_g$, and Q_d (as inputs of the model) and *DP* (as the output of the model). The goodness of fit was determined using some common statistical parameters, *i.e.* coefficient of determination (R^2), mean absolute percentage error (MAPE), and root mean squared error (RMSE). R^2 reveals whether or not regression accounts for the variation of data points: if the model accounts for all of the variations, R^2 is 1.0,

but if none of the variations are accounted for by the model, R^2 is zero [17, 19]. MAPE provides an intuitive way of judging the extent of errors [20] and can be considered as a measure of the model's accuracy. The RMSE indicates the precision of the model for different datasets [21]. Mathematical definitions and further descriptions of these parameters have been given elsewhere [21, 22]. Models which have high R^2, low MAPE, and low RMSE are more reliable.

Model robustness can be validated either by internal or external data. In external validation, the available dataset splits into two subsets: calibration and test sets. The model is built using the calibration set and then assessed using the test set [23]. If the dataset is quite small, as in the current work, the splitting of datasets may cause valuable information to be wasted. In these cases, internal validation methods have been proposed [24]. Cross validation is the most common technique of internal validation. In cross validation, one data point (or a subset containing several data points) is iteratively excluded from the dataset. Then the remaining data is used for developing the model and the predictive ability of the model is verified by the unknown compounds [25]. Cross validation methods can be divided into two branches: leave one-out (LOO CV) and *k*-fold cross validation (*k*-fold CV). In LOO CV, one single data point is removed as a tester while in *k*-fold CV the dataset is divided randomly into *k* groups and one group is left out as a tester in each run. In order to obtain a stable result for *k*-fold CV and to control the degrees of model flexibility, the procedure of splitting, calibrating, and testing of sub-models is repeated several hundred times. Finally a mean cross validated R^2, which is commonly known as Q^2, is derived [26, 27]. If the R^2 and Q^2 values for a new QSPR model are greater than 0.6 and 0.5, the model can be considered as a predictive tool [28].

On the basis of the values of R^2, Q^2, MAPE, and RMSE, the predictive ability of our new model has been assessed compared to the other methods. One of the best available methods, *i.e.* Kamlet-Jacobs (K-J) [4], has been used as a general technique for assessing the new model. Also the method of Zhang and Chang [10] and the outputs of BKWS-EOS (using full and partial consumption of Al and AN) have been used for explosives containing Al/AN.

3 Results and Discussion

On the basis of the oxygen content of explosives, a new reaction scheme containing six reactions has been proposed for the detonation of $C_aH_bN_cO_dF_eCl_fAl_g(NH_4NO_3)_h$ explosives [9]. In order to find a new and reliable MLR model for *DP*, the above reaction scheme has been tried for all of the 111 pure/mixed ideal/non-ideal

energetic materials that we considered. Examining the experimental values of *DP* and ρ_0 with different combinations of α, $\overline{MW}_g$, and Q_d showed that a reliable correlation can be established for predicting the *DP* in the form of Equation 2:

$$DP = 24.436\ \alpha\left(\overline{MW}_g\ Q_d\right)^{0.5}\ \rho_0^2 - 0.874 \tag{2}$$

where *DP*, α, $\overline{MW}_g$, Q_d, and ρ_0 are in GPa, mol·g^{-1}, g·mol^{-1}, kJ·g^{-1}, and g·cm^{-3}, respectively. Table 1 shows the predicted values of *DP* for 288 pure and mixed explosives compared to the experimental values and the results of the K-J method [4]. As seen in Table 1 both the MAPE and RMSE values for the Equation 2 are lower than for the K-J method [4], which shows the general acceptability of the new model for predicting the *DP* of various ideal or non-ideal energetic materials with different loading densities. A linear relationship between the predicted and experimental *DP* values was found (see Figure 1) for all 111 energetic materials. As shown in Figure 1, the R^2 value for Equation 2 is 0.9615, which is a reasonable value, and shows that the new model covers 96.15% of the variations. The R^2 value for the K-J method [4] is 0.8894. The accuracy of models can be determined by arranging the absolute percent errors (APE) into some groups.

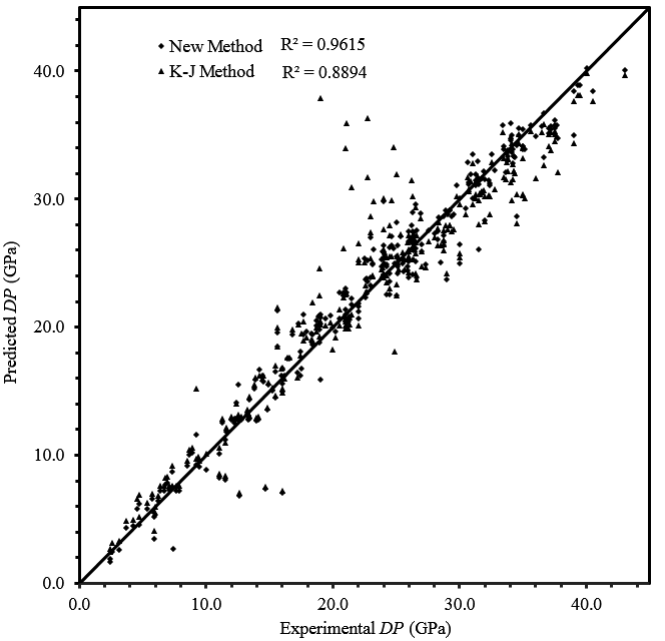

Figure 1. Plot of the Predicted DP values versus experimental data

Table 1. Detonation pressures (*DP* in GPa) for different classes of explosives

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
1	Acrylonitrile/TNM (1/1.25 molar)	1.380	15.6	[8]	21.3	36.6	21.6	38.2
2	AFX902	1.740	29.0	[31]	23.7	-18.2	24.2	-16.6
3	ALEX20	1.801	23.0	[8]	23.9	3.8	28.6	24.5
4	ALEX32	1.88	21.5	[8]	21.7	1.1	30.9	43.7
5	Amatol 80/20	1.46	7.4	[32]	2.7	-64.0	--	--
6	Amatol 50/50	1.55	16.0	[32]	7.1	-55.9	7.2	-54.8
		1.53	12.6	[33]	6.9	-45.6	7.0	-44.1
		1.58	14.67	[33]	7.4	-49.7	7.5	-48.8
7	AN/ADNT (2/1 molar)	1.64	26.1	[33]	26.7	2.2	27.0	3.5
8	AN/ADNT/Al (2/1/2.66 molar)	1.734	26.3	[33]	24.1	-8.2	30.2	14.8
9	AN/ADNT/EDD (3/1/1 molar)	1.607	24.2	[33]	24.9	2.9	25.4	5.1
10	AN/ADNT/ NQ(1.38/1/1.83 molar)	1.654	25.5	[33]	25.0	-2.0	25.8	1.2
11	AN/ADNT/RDX (1.38/1/1.5 molar)	1.717	31.7	[33]	30.5	-3.7	30.6	-3.5
12	AN/ADNT/RDX (5/1/1 molar)	1.699	24.0	[33]	29.8	24.1	30.1	25.2
13	AN/ADNT/RDX/ Al(5/1/1/3.3 molar)	1.752	25.0	[33]	28.2	12.6	32.0	27.8
14	AN/ADNT/TATB (2/1/1.3 molar)	1.765	28.3	[33]	26.8	-5.2	27.7	-2.1
15	ANFO 94.2/5.8	0.82	4.55	[33]	5.8	28.4	6.6	45.1
		0.84	4.74	[33]	6.2	30.3	6.9	46.2
16	ARX-2002	1.65	18.35	[34]	18.6	1.4	21.9	19.6
17	BTF	1.859	36.0	[35]	34.9	-3.0	31.7	-12.1
		1.85	34.0	[31]	34.6	1.7	31.4	-7.8
18	Comp A-3	1.59	26.0	[34]	25.1	-3.4	24.2	-6.7
		1.63	30.0	[2]	26.5	-11.8	25.5	-15.1
19	Comp B	1.73	29.2	[2]	29.1	-0.3	28.0	-4.2
		1.67	26.4	[34]	27.1	2.5	26.1	-1.3
20	Comp B, Grade A	1.717	29.5	[35]	28.8	-2.4	27.6	-6.3
		1.717	29.04	[33]	28.8	-0.8	27.6	-4.8
		1.713	29.4	[8]	28.7	-2.5	27.5	-6.4
21	Cyclotol-50/50	1.63	23.1	[7]	25.0	8.2	24.1	4.2
		1.627	23.11	[4]	24.9	7.8	24.0	3.8
22	Cyclotol-60/40 (or Comp B-3)	1.715	28.7	[35]	28.7	-0.1	27.5	-4.1
		1.680	28.3	[4]	27.5	-2.9	26.4	-6.6
		1.668	26.41	[4]	27.1	2.6	26.0	-1.4
23	Cyclotol-65/35	1.715	29.2	[4]	29.1	-0.3	28.0	-4.2
		1.715	28.9	[33]	29.1	0.7	28.0	-3.2

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
24	Cyclotol-75/25	1.76	31.6	[7]	31.6	-0.1	30.4	-3.7
		1.757	32.33	[33]	31.5	-2.7	30.3	-6.2
		1.648	27.59	[4]	27.6	-0.1	26.7	-3.3
		1.62	26.5	[7]	26.6	0.4	25.8	-2.7
25	Cyclotol-77/23	1.754	31.3	[36]	31.5	0.7	30.4	-2.8
		1.752	31.58	[33]	31.4	-0.5	30.3	-3.9
		1.743	31.3	[8]	31.1	-0.6	30.0	-4.1
26	Cyclotol-78/22	1.755	31.7	[33]	31.6	-0.2	30.5	-3.7
27	DATB	1.80	25.1	[7]	24.8	-1.3	25.6	2.1
		1.788	25.9	[8]	24.4	-5.6	25.3	-2.4
		1.78	25.1	[7]	24.2	-3.5	25.1	-0.1
28	Destex	1.68	17.5	[8]	16.7	-4.3	19.5	11.6
29	DNNC	1.82	34.0	[2]	35.9	5.6	34.9	2.7
30	1,2-DP	1.26	12.5	[31]	15.5	24.2	--	--
31	EARL-1	1.665	24.0	[33]	25.4	5.9	27.7	15.3
		1.595	23.0	[33]	23.3	1.1	25.4	10.4
32	EDC-11	1.782	31.5	[8]	31.2	-1.0	29.9	-5.0
33	EDC-24	1.776	34.2	[8]	32.8	-4.2	31.5	-7.9
34	EDD	1.563	21.0	[33]	21.4	1.8	22.6	7.5
35	EDNA	1.562	27.3	[4]	24.9	-8.9	24.7	-9.7
		1.532	26.59	[4]	23.9	-10.1	23.7	-10.8
36	FEFO	1.61	24.5	[31]	26.2	7.0	23.0	-6.0
		1.59	25.0	[35]	25.5	2.1	22.5	-10.2
37	H6 (or H-6)	1.76	24.5	[34]	22.6	-7.9	27.2	10.9
38	HBX-1	1.75	20.86	[33]	22.6	8.6	26.2	25.5
		1.72	22.04	[35]	21.8	-0.9	25.3	14.7
		1.712	22.04	[35]	21.6	-1.8	25.1	13.7
39	HMX	1.90	39.3	[8]	38.9	-1.1	38.1	-3.1
		1.90	39.5	[2]	38.9	-1.6	38.1	-3.6
		1.89	40.5	[31]	38.5	-5.0	37.7	-7.0
		1.89	39.0	[35]	38.5	-1.4	37.7	-3.4
		1.730	33.6	[36]	32.1	-4.5	31.6	-6.0
		1.60	28.0	[7]	27.3	-2.4	27.0	-3.6
		1.40	21.0	[7]	20.7	-1.4	20.7	-1.5
		1.20	16.0	[7]	15.0	-6.4	15.2	-5.1
		1.18	15.5	[31]	14.5	-6.7	14.7	-5.2
		1.00	11.0	[7]	10.1	-7.8	10.5	-4.1
		0.75	6.0	[7]	5.3	-11.3	5.9	-1.1
40	HMX/AP/EDNP (51/20/29)	1.67	23	[33]	27.0	17.4	27.4	19.3
41	HMX/EDNP (71/29)	1.66	27.0	[33]	26.4	-2.1	25.9	-3.9

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
42	HNAB	1.60	20.5	[35]	22.7	10.6	21.3	4.1
43	HNB	1.973	40.0	[33]	40.2	0.5	39.8	-0.5
		1.97	43.0	[31]	40.1	-6.8	39.7	-7.7
44	$HNO_3/H_2O/CH_3NO_2$(6.43/2.23/6.43 molar)	1.290	14.5	[8]	15.7	8.4	16.2	12.0
45	HNS	1.66	21.5	[31]	22.3	3.5	21.0	-2.6
		1.40	16.0	[31]	15.6	-2.6	14.9	-6.9
		1.20	11.5	[31]	11.2	-2.5	10.9	-4.8
		1.00	7.3	[31]	7.5	3.0	7.6	4.2
46	LX-01	1.31	15.6	[35]	18.5	18.6	18.5	18.7
47	LX-04	1.867	34.5	[33]	34.2	-0.8	30.4	-11.9
		1.866	35	[33]	34.2	-2.4	30.4	-13.3
		1.865	35.0	[35]	34.1	-2.5	30.3	-13.4
		1.858	35.13	[33]	33.9	-3.6	30.1	-14.3
		1.852	34.1	[36]	33.6	-1.3	29.9	-12.3
48	LX-07	1.85	37.73	[33]	34.7	-8.0	32.1	-14.9
49	LX-09	1.861	36.63	[33]	36.7	0.3	35.9	-2.1
		1.837	37.7	[35]	35.8	-5.1	35.0	-7.3
50	LX-10	1.860	37.5	[35]	36.2	-3.5	34.5	-7.9
		1.841	37.2	[33]	35.4	-4.7	33.8	-9.0
51	LX-14	1.833	37.0	[35]	35.1	-5.1	34.1	-7.8
52	LX-17	1.91	26.0	[31]	25.2	-3.0	26.0	0.1
		1.90	30.0	[35]	25.0	-16.8	25.8	-14.1
53	Minol-2	1.70	22.0	[37]	21.3	-3.4	26.5	20.5
54	NG	1.592	25.3	[4]	27.1	7.1	27.2	7.6
55	NM	1.159	14.8	[4]	13.5	-8.6	13.7	-7.5
		1.14	13.3	[4]	13.1	-1.8	13.3	-0.4
		1.135	12.5	[35]	12.9	3.5	13.1	5.1
		1.133	13.4	[33]	12.9	-3.9	13.1	-2.3
		1.13	12.5	[33]	12.8	2.5	13.0	4.2
		1.13	12.0	[31]	12.8	6.8	13.0	8.5
		1.128	14.1	[8]	12.8	-9.5	13.0	-8.0
		1.128	13.3	[33]	12.8	-4.0	13.0	-2.4
		1.128	12.8	[4]	12.8	-0.3	13.0	1.4
		1.125	14.0	[4]	12.7	-9.4	12.9	-7.8
56	NM/CT (50/50)	1.35	9.2	[8]	11.6	25.8	15.2	65.5
57	NM/TNM (1/0.071 molar)	1.197	13.8	[8]	15.2	10.3	15.5	12.2
58	NM/TNM (1/0.25 molar)	1.31	15.6	[33]	19.6	25.5	19.9	27.8
59	NM/TNM (1/0.50 molar)	1.397	16.8	[8]	19.4	15.8	19.8	18.1
60	NQ	1.72	24.5	[7]	24.2	-1.3	25.5	4.1

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
61	NTO/TNT 60/40	1.78	25.6	[34]	24.3	-5.0	25.4	-0.9
62	NTO/RDX/TNT 50/12/38	1.79	26.5	[34]	26.1	-1.4	26.6	0.5
63	Octol-77.6/22.4	1.821	34.18	[33]	33.9	-0.9	32.7	-4.3
64	Octol-76.3/23.7	1.81	33.8	[7]	33.4	-1.3	32.2	-4.8
		1.809	34.3	[8]	33.3	-2.9	32.1	-6.3
65	Octol-76/24	1.81	34.3	[2]	33.3	-2.8	32.2	-6.3
66	Octol-75/25	1.81	34.37	[34]	33.2	-3.3	32.1	-6.7
		1.803	31.4	[4]	33.0	5.1	31.8	1.3
		1.8	30.65	[33]	32.9	7.3	31.7	3.4
67	Octol-60/40	1.80	32.0	[7]	31.5	-1.5	30.2	-5.5
68	PATO	1.94	34.5	[38]	28.6	-17.0	28.1	-18.6
69	PBX-9007	1.60	26.5	[35]	25.2	-5.0	24.2	-8.8
70	PBX-9010	1.783	32.8	[35]	32.2	-1.8	30.8	-6.2
		1.781	31.9	[8]	32.1	0.8	30.7	-3.8
71	PBX-9011	1.767	29.8	[8]	31.1	4.4	30.2	1.3
		1.767	32.4	[35]	31.1	-4.0	30.2	-6.8
72	PBX-9404	1.846	37.5	[33]	35.8	-4.6	35.3	-5.9
		1.846	35.6	[33]	35.8	0.5	35.3	-0.9
		1.845	33.4	[33]	35.7	7.0	35.2	5.5
		1.844	37.2	[33]	35.7	-4.0	35.2	-5.4
		1.844	36.5	[8]	35.7	-2.2	35.2	-3.6
		1.840	37.5	[35]	35.6	-5.2	35.0	-6.6
		1.84	37.0	[33]	35.6	-3.9	35.0	-5.3
		1.84	34.7	[33]	35.6	2.5	35.0	1.0
		1.60	28.7	[35]	26.7	-7.1	26.5	-7.7
		0.969	9.2	[8]	9.2	0.3	9.7	5.6
73	PBX-9407	1.60	28.7	[35]	26.4	-8.0	26.0	-9.4
74	PBX-9502	1.894	28.5	[8]	25.1	-12.0	26.4	-7.5
75	PBXN-1	1.77	24.5	[8]	23.6	-3.7	28.0	14.2
76	Pentolite-50/50	1.68	25.1	[7]	26.4	5.0	25.6	1.8
		1.68	24.6	[34]	26.4	7.1	25.6	3.9
		1.67	26.4	[4]	26.0	-1.4	25.3	-4.3
		1.66	24.1	[33]	25.7	6.7	25.0	3.5
		1.644	25.63	[33]	25.2	-1.7	24.5	-4.5
		1.644	25.2	[33]	25.2	0.0	24.5	-2.9
77	Pentolite-45/55	1.677	23.96	[4]	25.9	7.9	25.0	4.5
78	Pentolite-40/60	1.673	23.83	[4]	25.3	6.2	24.5	2.8
79	Pentolite-35/65	1.668	23.85	[4]	24.7	3.6	23.9	0.4
80	PETN	1.77	35.0	[4]	33.9	-3.2	33.2	-5.1
		1.77	33.5	[33]	33.9	1.1	33.2	-0.9

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
80	PETN (continuation)	1.762	33.7	[33]	33.6	-0.4	32.9	-2.4
		1.76	31.0	[34]	33.5	8.0	32.8	5.9
		1.703	30.75	[33]	31.3	1.8	30.7	0.0
		1.70	30.7	[7]	31.2	1.6	30.6	-0.2
		1.67	31.0	[4]	30.1	-3.0	29.6	-4.6
		1.67	30.0	[35]	30.1	0.2	29.6	-1.5
		1.648	30.5	[4]	29.3	-4.1	28.8	-5.6
		1.60	26.6	[7]	27.5	3.5	27.1	2.0
		1.597	26.37	[33]	27.4	4.0	27.0	2.5
		1.568	23.99	[4]	26.4	10.1	26.1	8.6
		1.538	22.47	[4]	25.4	12.9	25.1	11.6
		1.50	24.0	[31]	24.1	0.4	23.8	-0.6
		1.45	20.8	[7]	22.5	7.9	22.3	7.1
		1.38	17.3	[33]	20.3	17.1	20.2	16.7
		1.26	16.0	[31]	16.7	4.6	16.8	5.2
		1.23	13.87	[33]	15.9	14.7	16.0	15.6
		0.99	8.7	[33]	10.0	14.9	10.4	19.4
		0.95	8.5	[33]	9.1	7.5	9.6	12.5
		0.93	7.33	[33]	8.7	19.0	9.2	25.1
		0.885	6.95	[33]	7.8	12.5	8.3	19.4
		0.88	6.8	[7]	7.7	13.5	8.2	20.7
		0.50	2.4	[8]	1.9	-20.8	2.6	10.4
		0.48	2.4	[7]	1.7	-29.9	2.4	1.8
81	PYX	1.75	24.2	[2]	24.8	2.3	24.0	-0.7
82	RDX	1.80	39.0	[4]	35.0	-10.2	34.4	-11.9
		1.80	34.7	[8]	35.0	0.9	34.4	-1.0
		1.8	34.1	[33]	35.0	2.7	34.4	0.7
		1.77	33.8	[2]	33.8	0.1	33.2	-1.7
		1.767	33.8	[35]	33.7	-0.2	33.1	-2.1
		1.762	32.5	[33]	33.5	3.2	32.9	1.3
		1.755	36.6	[4]	33.3	-9.1	32.7	-10.8
		1.72	31.3	[7]	31.9	1.9	31.4	0.2
		1.72	30.85	[33]	31.9	3.4	31.4	1.7
		1.64	26.9	[4]	28.9	7.5	28.5	6.0
		1.63	28.37	[4]	28.6	0.7	28.2	-0.7
		1.60	26.3	[7]	27.5	4.5	27.1	3.2
		1.6	26	[33]	27.5	5.7	27.1	4.4
		1.59	28.7	[4]	27.1	-5.4	26.8	-6.6
		1.46	21.1	[7]	22.7	7.8	22.6	7.1
		1.46	20.8	[33]	22.7	9.3	22.6	8.7

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
82	RDX (continuation)	1.40	21.3	[7]	20.8	-2.1	20.8	-2.4
		1.29	16.6	[7]	17.6	5.8	17.6	6.3
		1.29	16.40	[33]	17.6	7.1	17.6	7.6
		1.216	14.89	[33]	15.5	4.2	15.7	5.3
		1.20	15.2	[7]	15.1	-0.8	15.3	0.4
		1.173	13.44	[33]	14.4	6.9	14.6	8.5
		1.13	13.25	[33]	13.3	0.2	13.5	2.2
		1.1	12.2	[7]	12.5	2.7	12.8	5.2
		1.1	11.27	[33]	12.5	11.2	12.8	13.8
		1.07	11.6	[33]	11.8	1.8	12.1	4.6
		1.0	8.9	[7]	10.2	14.7	10.6	19.1
		0.95	9.46	[33]	9.1	-3.5	9.6	1.2
		0.70	4.72	[33]	4.6	-3.5	5.2	10.1
		0.56	3.16	[33]	2.6	-17.7	3.3	5.2
83	RDX/Al (90/10)	1.68	24.6	[7]	27.1	10.2	29.9	21.6
84	RDX/Al (80/20)	1.73	22.7	[7]	25.2	10.9	31.7	39.8
85	RDX/Al (70/30)	1.79	21.0	[7]	23.0	9.7	34.0	61.8
86	RDX/Al (60/40)	1.84	21.1	[7]	20.0	-5.1	35.9	70.1
87	RDX/Al (50/50)	1.89	19.0	[7]	15.9	-16.4	37.9	99.3
88	RDX/Exon (90.1/9.9)	1.786	32.0	[8]	28.4	-11.3	28.3	-11.6
89	RDX/TFNA (65/35)	1.754	32.4	[8]	31.3	-3.5	28.8	-11.0
90	RX36AH	1.830	33.5	[31]	34.1	1.9	31.7	-5.4
91	RX41AB	1.857	35.0	[31]	35.5	1.3	34.0	-2.9
92	RX27AD	1.638	20.0	[31]	20.0	-0.1	18.2	-8.9
93	RX45AA	1.752	25.0	[31]	22.5	-10.2	23.3	-6.6
94	RX47AA	1.823	26.0	[31]	26.7	2.7	25.5	-1.8
95	RX48AA	1.848	26.3	[31]	29.0	10.1	26.9	2.1
96	TATB	1.895	31.5	[8]	26.1	-17.3	28.0	-11.1
		1.847	25.9	[4]	24.7	-4.6	26.6	2.7
		1.83	26.0	[31]	23.9	-8.1	25.9	-0.2
		1.51	17.46	[4]	16.2	-7.0	17.8	1.8
97	Tetryl	1.70	26.3	[4]	26.5	0.9	25.3	-3.8
		1.681	27.0	[36]	25.9	-4.0	24.7	-8.4
		1.68	23.9	[7]	25.9	8.4	24.7	3.3
		1.614	22.64	[4]	23.8	5.3	22.8	0.7
		1.61	22.6	[7]	23.7	4.9	22.7	0.4
		1.36	14.2	[7]	16.7	17.4	16.2	14.0
98	TFENA	1.523	17.4	[8]	18.1	4.2	--	--
99	TFNA	1.692	24.9	[8]	24.9	0.2	18.1	-27.3
100	TNETB	1.69	26.5	[4]	29.6	11.6	29.3	10.7

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
101	TNETB/Al (90/10)	1.75	26.2	[7]	27.9	6.6	31.5	20.0
102	TNETB/Al (80/20)	1.82	24.8	[7]	26.1	5.3	34.0	37.2
103	TNETB/Al (70/30)	1.88	22.7	[7]	23.5	3.7	36.3	59.9
104	TNM	1.65	15.5	[31]	16.5	6.4	17.0	9.9
		1.638	15.9	[33]	16.2	2.1	16.8	5.6
105	TNT	1.64	21.0	[7]	21.0	-0.2	20.4	-2.8
		1.64	17.7	[33]	21.0	18.4	20.4	15.3
		1.64	19.0	[8]	21.0	10.3	20.4	7.4
		1.638	19.8	[33]	20.9	5.6	20.4	2.8
		1.637	18.9	[32]	20.9	10.4	20.3	7.5
		1.636	18.84	[33]	20.9	10.7	20.3	7.8
		1.632	21.3	[4]	20.7	-2.6	20.2	-5.1
		1.632	19	[33]	20.7	9.2	20.2	6.4
		1.630	22.0	[4]	20.7	-5.9	20.2	-8.4
		1.630	21.0	[35]	20.7	-1.5	20.2	-4.0
		1.63	20.5	[31]	20.7	0.9	20.2	-1.7
		1.63	19.44	[33]	20.7	6.4	20.2	3.7
		1.622	18.7	[4]	20.5	9.4	20.0	6.6
		1.62	21.0	[4]	20.4	-2.7	19.9	-5.2
		1.62	21.2	[4]	20.4	-3.6	19.9	-6.1
		1.61	18.7	[34]	20.2	7.8	19.7	5.2
		1.595	18.9	[33]	19.8	4.6	19.3	2.1
		1.59	20.2	[4]	19.6	-2.7	19.2	-5.0
		1.59	17.9	[4]	19.6	9.8	19.2	7.2
		1.583	18.3	[33]	19.5	6.4	19.0	3.9
		1.58	18.4	[33]	19.4	5.4	18.9	2.9
		1.58	17.7	[33]	19.4	9.5	18.9	7.0
		1.45	16.2	[4]	16.2	0.0	16.0	-1.5
		1.45	14.4	[7]	16.2	12.4	16.0	10.8
		1.36	12.4	[7]	14.1	14.0	14.0	13.2
		1.30	12.3	[4]	12.8	4.4	12.8	4.2
		1.14	9.4	[4]	9.7	2.9	9.9	4.9
		1.051	11.5	[4]	8.1	-29.6	8.4	-27.1
		1.061	11.0	[8]	8.3	-24.9	8.5	-22.4
		1.001	7.096	[33]	7.3	2.3	7.6	7.1
		1.00	7.9	[4]	7.2	-7.7	7.6	-3.3
		1.00	7.6	[4]	7.2	-5.1	7.6	-0.6
		1.00	6.7	[7]	7.2	8.1	7.6	13.2
		1.00	6.4	[4]	7.2	13.2	7.6	18.5
		0.96	5.74	[33]	6.6	15.1	7.0	21.8

No.	Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]			
					New method	% dev.	K-J method	% dev.
105	TNT (continuation)	0.95	6.22	[4]	6.5	3.7	6.8	10.1
		0.91	5.384	[33]	5.8	8.6	6.3	16.7
		0.866	5.889	[33]	5.2	-11.5	5.7	-3.4
		0.81	4.213	[33]	4.5	5.7	5.0	18.2
		0.80	3.7	[7]	4.3	16.8	4.9	31.2
		0.732	5.9	[8]	3.5	-41.1	4.1	-31.1
		0.642	2.62	[33]	2.5	-5.7	3.1	19.4
106	TNT (Liquid)	1.447	17.2	[8]	16.5	-4.3	16.0	-6.7
107	TNT/Al (78.3/21.7)	1.80	18.9	[7]	20.2	6.7	24.6	30.1
108	TNT/Al (80/20)	1.72	18.9	[39]	18.8	-0.5	22.4	18.8
109	Toluene/NM (14.5/85.5)	1.088	10.0	[8]	8.9	-11.1	10.1	1.4
110	Torpex	1.81	23.2	[40]	26.1	12.5	29.8	28.4
111	X-0489	1.72	24.2	[41]	22.6	-6.6	23.5	-2.8
		1.71	22.6	[34]	22.3	-1.2	23.2	2.9
MAPE					**7.1**		**9.9**	
RMSE					**1.8**		**3.1**	

Figure 2 shows the plot of APE values for the new model and the K-J method [4]. If, for example, an APE of 6 is used as the measure, it can be seen that the new model predicts 173 data points within this range. In other word, more than 60% of predictions of our new model are very accurate. In 142 cases (*i.e.* about 50%), the predictions of the K-J method [4] show APE values in this range.

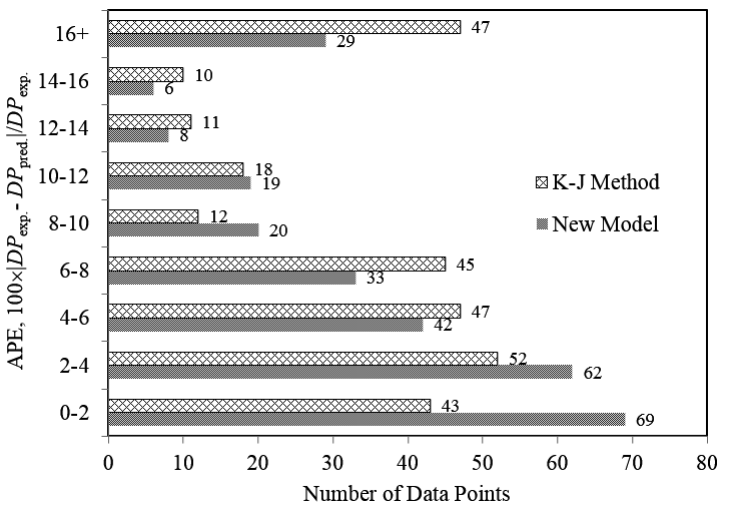

Figure 2. Plot of the range of absolute percent errors

The goodness-of-fit is shown by R^2 but in order to assess the goodness-of-prediction, one need to calculate the Q^2 values through cross-validation procedure. Generally Q^2 values are smaller than R^2 but in a well-behaved model, Q^2 and R^2 values do not have a significant difference [29]. If the Q^2 values are also independent of partition size and close to R^2, the robustness of the model can be inferred [30]. Different Q^2 values, *i.e.* the coefficients of determination for LOO-CV (Q^2_{LOO}), 5-fold CV (Q^2_{5CV}) and 10-fold CV (Q^2_{10CV}), were calculated for the new model. As shown in Table 2, the R^2, Q^2_{LOO}, Q^2_{5CV}, and Q^2_{10CV} values are significantly greater than the threshold values, *i.e.* 0.6 for R^2 and 0.5 for Q^2 respectively, so the new model is a reliable predictive model. Moreover, all values of Q^2 are same as R^2 and are near each other, so the new model is a well-behaved and robust model. Also as shown in Table 2, the MAPE and RMSE values of cross validation datasets are very close or even equal to the MAPE and RMSE of model, respectively. So the new model is precise and accurate.

Table 2. Coefficient of determinations, MAPE values, and RMSE values of cross validations

Parameter	Whole model	Cross validation		
		Leave one-out CV	5-fold CV [a]	10-fold CV [a]
Coefficients of determination	0.9615 [b]	0.9612 [c]	0.9597 [d]	0.9578 [e]
MAPE	7.1 [f]	7.2 [g]	7.1 [h]	7.2 [i]
RMSE	1.8 [j]	1.8 [k]	1.8 [l]	1.7 [m]

[a] The averages of 1000 runs; [b] R^2; [c] Q^2_{LOO}; [d] Q^2_{5CV}; [e] Q^2_{10CV}; [f] $MAPE_{Model}$; [g] $MAPE_{LOO}$; [h] $MAPE_{5CV}$; [I] $MAPE_{10CV}$; [j] $RMSE_{Model}$; [k] $RMSE_{LOO}$; [l] $RMSE_{5CV}$; [m] $RMSE_{5CV}$.

Reliable prediction of *DP* for non-ideal explosives has great importance, so as a further assessment of Equation 2, comparisons were performed with the other predictive methods. In Table 3, the predicted values of *DP* for non-ideal explosives containing Al are compared to the results of Zhang and Chang's method [10] and the outputs of BKWS-EOS, in both full and partial equilibriums [7]. As shown in Table 3, the results of the new model are in good agreement with the experimental detonation pressures. Comparison of the MAPE and RMSE values for the different models prove this assertion.

Table 3. Detonation pressures (*DP* in GPa) for non-ideal explosives

Explosive	ρ_0 [g·cm^{-3}]	*DP* [GPa]	Ref.	Predicted values for *DP* [GPa]							
				New method	% dev.	BKWS, full	%Dev.	BKWS, partial	% dev.	Ref. [10]	% dev.
ALEX20	1.801	23.0	[8]	23.9	3.8	--	--	--	--	25.9	12.8
ALEX32	1.88	21.5	[8]	21.7	1.1	--	--	--	--	23.2	8.0
Destex	1.68	17.5	[8]	16.7	-4.3	--	--	--	--	17.5	-0.2
H6 (or H-6)	1.76	24.5	[34]	22.6	-7.9	21.5	-12.2	21.6	-11.8	23.3	-4.8
HBX-1	1.712	22.04	[35]	21.6	-1.8	21.1	-4.3	20.9	-5.2	24.4	10.8
Minol-2	1.70	22.0	[37]	21.3	-3.4	21.1	-4.1	14.4	-34.6	--	--
RDX/Al (90/10)	1.68	24.6	[7]	27.1	10.1	26.4	7.3	25.7	4.5	25.9	5.3
RDX/Al (80/20)	1.73	22.7	[7]	25.2	10.9	24.4	7.5	23.7	4.4	23.6	3.9
RDX/Al (70/30)	1.79	21.0	[7]	23.0	9.7	20.5	-2.4	21.2	1.0	21.3	1.5
RDX/Al (60/40)	1.84	21.1	[7]	20.0	-5.1	15.6	-26.1	17.4	-17.5	18.6	-11.9
RDX/Al (50/50)	1.89	19.0	[7]	15.9	-16.4	12.0	-36.8	11.9	-37.4	15.7	-17.2
TNETB/Al (90/10)	1.75	26.2	[7]	27.9	6.5	26.9	2.7	25.8	-1.5	--	--
TNETB/Al (80/20)	1.82	24.8	[7]	26.1	5.3	25.6	3.2	24.4	-1.6	--	--
TNETB/Al (70/30)	1.88	22.7	[7]	23.5	3.7	21.9	-3.5	21.9	-3.5	--	--
TNT/Al (78.3/21.7)	1.80	18.9	[7]	20.2	6.7	18.3	-3.2	18.7	-1.1	17.0	-10.1
TNT/Al (80/20)	1.72	18.9	[39]	18.8	-0.5	--	--	--	--	18.26	-3.4
Torpex	1.81	23.2	[40]	26.1	12.5	--	--	--	--	27.1	16.9
MAPE (Data Points)				**7.3 (12)**[a] **7.0 (13)**[b]		**9.4 (12)** --		10.3 (12) --		-- 8.2 (13)	
RMSE (Data Points)				**1.8 (12)**[a] **1.8 (13)**[b]		**2.9 (12)** --		3.3 (12) --		-- 2.1 (13)	

[a] Compared to the outputs of BKWS-EOS; [b] Compared to the method of Zhang and Chang.

4 Conclusion

The detonation pressure of explosives is an important parameter defining the performance of explosives. A new correlation has been presented for the calculation of the *DP* values of pure as well as mixtures of ideal and non-ideal explosives. The needed inputs are ρ_0 and $\Delta_f H^{\grave{e}}$ (c). The other data needed, *i.e.* Q_d, α, and $\overline{MW}_g$, are calculated on the basis of a new reaction scheme. The new approach can be easily used for different CHNO, CHNOFCl, CHNOFClAlAN explosives, as well as different PBXs. Internal validation of the model has been performed in LOO-CV, 5-fold CV, and 10-fold CV modes and different values of Q^2, *i.e.* Q^2_{LOO}, Q^2_{5CV} and Q^2_{10CV} values were compared with the model's R^2. The RMSE and MAPE values for cross validation datasets were also compared with the RMSE and MAPE of the model. Moreover, different statistical parameters, *i.e.* R^2, RMSE, MAPE values, were used to compare the new method with the outputs of BKWS-EOS in full and partial modes as well as other predictive methods. The results showed that the new model is a well-defined, robust, precise, and accurate model which provides reliable prediction of detonation pressures for different pure as well as mixtures of ideal or non-ideal explosives with acceptable deviations.

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