

# Predicting Detonation Performance of CHNOFCl and Aluminized Explosives

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**Abstract:** A new “hand-calculated” method is introduced for prediction of detonation pressure of explosive and mixture of explosives with general formula CHNOFClAl. Suitable decomposition paths are used to estimate heat of detonation and detonation pressure. These decomposition paths are based on the distribution of oxygen atoms between carbon and hydrogen atoms as well as the degree of oxidation of aluminum. For CHNOFCl explosives, it is shown that the predicted detonation pressures with the

new method are more reliable with respect to one of the best available empirical methods for loading densities greater than or equal  $0.8 \text{ g cm}^{-3}$ . Since aluminized explosives have non-ideal behavior, the new method does not require using full or partial oxidation of aluminum, which is usually required by a computer code. The predicted results of the new model also provide more reliable results than outputs of complex computer code with the BKWS equation of state.

**Keywords:** Detonation performance · Decomposition reaction · Heat of detonation · CHNOFClAl explosive · Loading density

## 1 Introduction

Non-ideal explosives such as aluminized explosives are often poorly modeled by Chapman-Jouguet (C-J) theory because the C-J assumption of instantaneous thermodynamic equilibrium breaks down. They have significantly different detonation properties than predicted by equilibrium, one-dimensional and steady state calculations. Physical separation of the fuel and oxidizer in aluminized explosives results in extended chemical reaction zones. Two characteristics of non-ideal explosives contain the high degree of inhomogeneity and the secondary exothermic reactions occurring in the detonation products expanding behind the detonation zone. Furthermore, diffusion has a major role in experimentally determined detonation properties and the amount of reacted material is a function of reaction zone length.

Detonation pressure is the important parameter that has been regarded as one of the principal measures of performance of detonating explosive for many years. The determination of the time-independent state of chemical equilibrium, which is defined in accordance with the C-J condition, has historically special attention. Due to presence of the nonsteady-state nature of the detonation wave, it is reasonable to expect the calculated and experimental C-J pressures to differ by 10 to 20% [1]. For aluminized explosives, detonation pressures are significantly different from those predicted by equilibrium, one dimensional and steady state calculations. Moreover, addition of aluminum to explosives can increase explosive performance through raising reaction temperature and prolongs the reaction time.

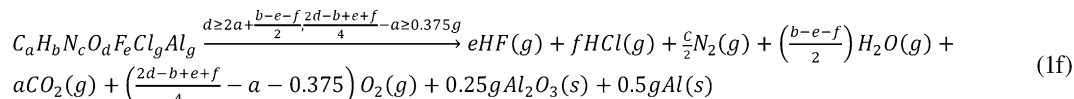
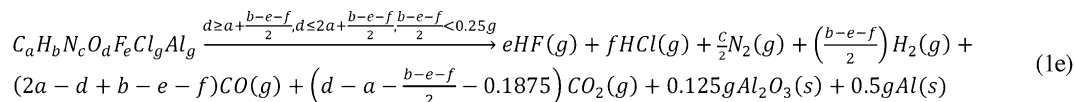
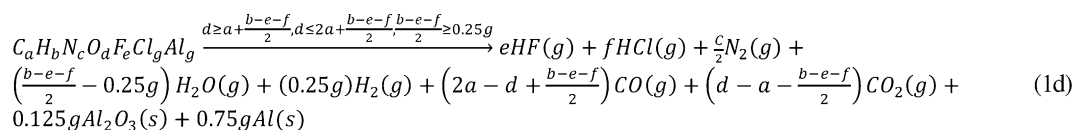
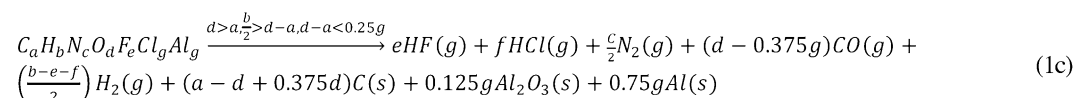
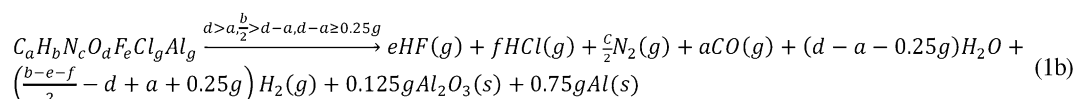
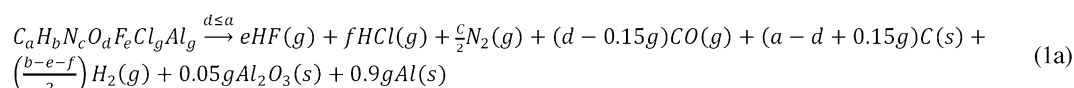
In contrast to CHNOFCl explosives, where different approaches have been developed to predict their detonation performance, there are several methods to predict detonation performance of aluminized explosives through the molecular structure of explosive component [2–8]. Application of these methods for a wide range of ideal and non-ideal explosives is rather limited because deviations of these correlations may be large for some energetic compounds containing unusual molecular fragments. Moreover, these methods cannot be used for some pure and mixture of high explosives containing high content of oxygen atoms. The purpose of this work is to introduce an easy to handle general correlation for calculating detonation pressure of any pure and mixture of CHNOFCl explosives as well as aluminized explosives at loading density greater than or equal  $0.8 \text{ g cm}^{-3}$ . Several decomposition paths are introduced to specify detonation products on the basis of oxygen content of explosive and extent of reaction of aluminum with products. For CHNOFCl and aluminized explosives, the predicted detonation pressures are also compared with empirical well-known method of Kamlet-Jacobs (K-J) [9] and the computed results of the BKWS equation of state, respectively [10].

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## 2 Materials and Method

For prediction of detonation properties of aluminized explosives by using a thermodynamic computer code, as a simple approximation, partial equilibrium can be used rather than a complex reacting mechanism. However, thermodynamic calculations of detonation parameters are carried out by assuming a certain degree of oxidation of aluminum because it is not obvious what degree of aluminum will be oxidized in the C-J point. Inert aluminum atoms in form of solid, liquid, or gaseous were included in the product species data base to prevent reaction of aluminum with oxygen or other reactive species. The amount of the react-

terials stays a major unresolved problem. For various explosives with general formula  $C_aH_bN_cO_dF_eCl_f$  over a wide range of loading density, four decomposition pathways were assumed to predict their detonation performance [2]. It was indicated that oxygen content of the explosive can control degree of aluminum oxidation [2–8]. Thus, on the basis of previous studies for decomposition paths of  $C_aH_bN_cO_dF_eCl_f$  and aluminized explosives, it can be assumed that all nitrogen atoms go to  $N_2$ , fluorine atoms to HF, chlorine atoms to HCl, while a portion of the oxygen atoms form  $H_2O$ , carbon atoms preferentially are oxidized to CO rather than  $CO_2$  and part of aluminum are oxidized to  $Al_2O_3$  according to the following pathways in going from oxygen-lean to oxygen-rich explosives:



ed initial aluminum is specified in order to invoke partial equilibrium. Prevention of the formation of aluminum oxide ( $Al_2O_3$ ), by reaction of aluminum with composite explosives such as HMX, causes an increase in the number of gaseous products. More condensed  $Al_2O_3$  is produced by assuming complete equilibrium because the higher temperature is a result of the large negative heat of formation of  $Al_2O_3$ . Since complete equilibrium force oxygen to react with aluminum rather than carbon, a hot, fuel-rich gas phase and more solid carbon can be formed.

The equilibrium composition of the products can be determined through (i) experimental measurement; (ii) thermochemical equilibrium, and (iii) by suggesting an appropriate detonation reaction. However, accurate estimation of composition of decomposition products for energetic ma-

Experiments for determining the performance of most explosives reveal that detonation pressure is roughly proportional to the number of moles of gaseous products, heat of detonation, and square of loading density [2, 11]. The heat of detonation can be determined from the heats of formation of reactants and decomposition products of the explosive as follows:

$$Q_{det} \cong - \frac{[\Delta_f H^\theta(\text{products}) - \Delta_f H^\theta(c)]}{\text{formula mass of explosive}} \quad (2)$$

where  $\Delta_f H^\theta(\text{products})$  [ $J \text{ mol}^{-1}$ ],  $\Delta_f H^\theta(c)$  [ $J \text{ mol}^{-1}$ ], and  $Q_{det}$  [ $J \text{ kg}^{-1}$ ] are the heats of formation of detonation products, the condensed phase heat of formation of the explosive, and the heat of detonation, respectively. Table 1 contains

the basic parameters for various pure, mixtures of explosives and composite aluminized explosives. Experimental data of detonation pressures at specified loading densities are also given in Table 2, Table 3, and Table 4. As shown in Figure 1, the measured detonation pressure vs.  $n_g(\bar{M}_g Q_{\text{det}})^{0.5} \rho_0^2$  shows linear correlation of the form:

$$P = (7.884 \times 10^5 \text{ GPa m}^6 \text{ kg}^{-1} \text{ mol}^{-1} \text{ J}^{-0.5}) n_g (\bar{M}_g Q_{\text{det}})^{0.5} \rho_0^2 - 1.484 \text{ GPa} \quad (3)$$

where  $P$  is the detonation pressure in GPa,  $n_g$  is the number of moles of gaseous products of detonation per g of explosive,  $\bar{M}_g$  is the average molecular mass of gaseous products, and  $\rho_0$  is the loading density.

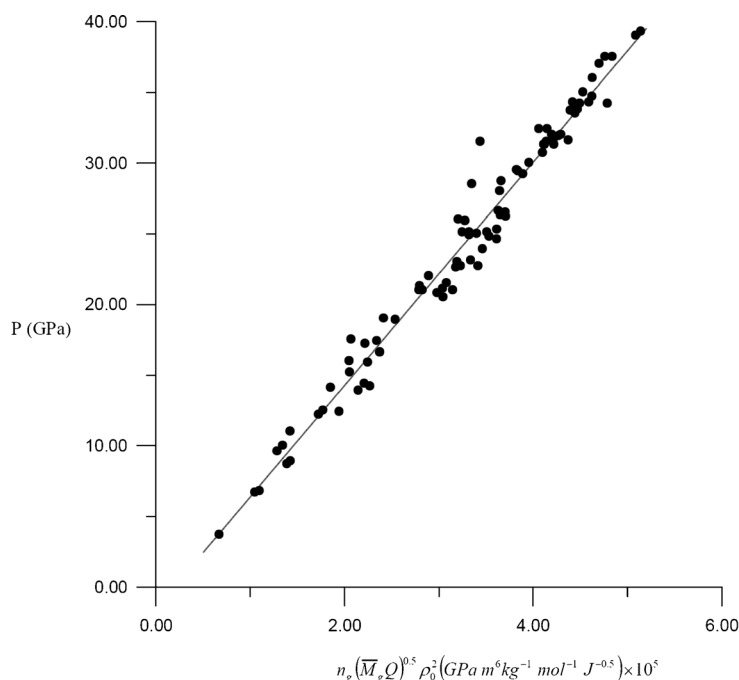
### 3 Results and Discussion

Comparison of the calculated results with experimental data may be taken as appropriate validation test of Equation (3) for use with different types of CHNOFCl explosives. For CHNO and CHNOFCl explosives, the calculated detonation pressures of well-known pure and mixed explosives are given in Table 2 and Table 3, respectively. The predicted results for CHNO explosives are also compared with the estimated values of K-J method [9]. As seen in Table 2, Equation (3) provides surprisingly very good agreement with experimental data as compared to K-J method.

For aluminized explosives, the calculated detonation pressures are also given in Table 4 and compared with the results from the BKWS-EOS using full and partial equilibrium [10]. It was assumed that only 50% of aluminum is in-

**Table 1.** Parameters used in Equation (3).

Explosive	$\Delta_f H^\circ \times 10^3$ [J mol <sup>-1</sup> ]	$Q$ [J kg <sup>-1</sup> ]	$n_g \times 10^3$ [mol kg <sup>-1</sup> ]	$\bar{M}_g \times 10^3$ [kg mol <sup>-1</sup> ]	Explosive	$\Delta_f H^\circ \times 10^3$ [J mol <sup>-1</sup> ]	$Q$ [J kg <sup>-1</sup> ]	$n_g \times 10^3$ [mol kg <sup>-1</sup> ]	$\bar{M}_g \times 10^3$ [kg mol <sup>-1</sup> ]
HMX	75.0 [12]	5.02	0.0405	24.67	PENTOLITE	-82.1	3.91	0.0416	24.02
RDX	61.5 [10]	5.04	0.0405	24.67	LX-09	8.4	4.84	0.0410	24.36
TNT	-67.1 [12]	2.65	0.0441	21.5	LX-04	-90.0	4.04	0.0425	23.54
PETN	-535.9 [10]	5.79	0.0348	28.73	HBX 1	-10.6	3.26	0.0394	19.39
Tetryl	20.1 [12]	3.61	0.0418	23.92	90RDX/10Al	24.9	4.97	0.0365	24.06
DATB	-98.8 [12]	2.32	0.0453	22.09	80RDX/20Al	22.1	4.91	0.0327	23.35
NG	-371.0 [12]	6.27	0.0319	31.31	70RDX/30Al	19.4	4.86	0.0284	22.32
TNM	54.4 [10]	2.29	0.0306	32.67	60RDX/40Al	16.6	4.78	0.0243	21.01
TATB	-139.8 [12]	1.98	0.0465	21.50	50RDX/50Al	13.9	4.78	0.0205	19.16
NM	-113.5 [12]	3.93	0.0492	20.33	TNTEB/AL(90/10)	-116.2	5.82	0.028	31.37
FEFO	-743.2 [10]	5.27	0.0344	29.09	TNTEB/AL(80/20)	-103.2	5.66	0.025	30.44
TFNA	-766.3 [4]	3.10	0.0435	23.00	TNTEB/AL(70/30)	-90.4	5.51	0.0218	29.11
TFENA	-695.1 [4]	2.45	0.0417	24.00	TNT/AL(78.3/21.7)	-21.6	2.61	0.0333	21.26
65/35 RDX/TFNA	-824.5	4.26	0.0410	24.36	ALEX20	-7.6	3.42	0.0381	19.56
PBX-9010	-33.0	4.55	0.0399	25.05	ALEX32	-9.3	3.77	0.0342	17.26
90.54/9.46 HMX/Exon	-1027.5	4.57	0.0409	24.45	Destex	-34.4	2.32	0.0347	19.33
PBX-9502	-87.1	1.96	0.0452	21.93	Cyclotol	13.9	4.35	0.0424	23.60
90.1/9.9 RDX/Exon	-195.6	4.43	0.0410	24.42	EDC-11	4.5	3.80	0.0449	22.24
Cyclotol 77/23 RDX/TNT	-778.8	4.35	0.0424	23.61	EDC-24	18.3	4.25	0.0493	22.34
Lx-10	-13.1	4.73	0.0414	24.18	Liquid TNT	-53.3 [4]	2.69	0.0441	21.50
Composition B	4.2	3.95	0.0434	23.05	14.5Toluene/ 85.5Nitromethane	-130.3	2.19	0.0593	16.84
Octol	11.5	4.31	0.0424	23.58					
PBX-9407	3.4	5.01	0.0409	24.45					
HNAB	284.3 [10]	3.57	0.0398	25.11					
LX-14	6.3	4.50	0.0428	23.39					
PBX-9011	-17.0	3.87	0.0454	22.00					
BTF	602.9 [10]	5.02	0.0357	28.00					
Cyclotol 50/50 RDX/TNT	0.0	3.55	0.0445	22.47					
Cyclotol 65/35 RDX/TNT	8.3	4.00	0.0433	23.09					
Cyclotol 75/25 RDX/TNT	13.9	4.30	0.0464	21.56					
Cyclotol 77/23 RDX/TNT	15.0	4.36	0.0424	23.59					
Cyclotol 78/22 RDX/TNT	15.5	4.39	0.0423	23.65					
COMP B-3	5.6	3.83	0.0438	22.82					
OCTOL 78/22	13.5	4.36	0.0423	23.63					
OCTOL 76/23	12.8	4.32	0.0424	23.58					
OCTOL 60/40	4.1	3.84	0.0437	22.90					
PENTOLITE	-100.1	3.73	0.0416	24.02					



**Figure 1.** The measured detonation pressure vs.  $n_g(\bar{M}_g Q)^{0.5} \rho_0^2$  ( $\text{GPa m}^6 \text{ kg}^{-1} \text{ mol}^{-1} \text{ J}^{-0.5}$ )  $\times 10^5$  for various explosive given in Table 2, Table 3, and Table 4.

teracting with combustion products in the case of partial equilibrium. As indicated in Table 4, the “hand calculated” detonation pressures of Equation (3) show surprisingly very good agreement with experimental data as compared to the computed results of complicated computer programs. Thus, Equation (3) requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical property of explosive and detonation products except  $\Delta_f H^0(c)$  at a specified density  $\rho_0$ .

## 4 Conclusions

A simple general correlation was introduced for desk calculation of detonation pressure of the secondary CHNOFCIAL explosives. Though measured data of detonation pressures are rare in open literature, predicted detonation pressures from the new method are consistent with reported values from different sources. Decomposition reactions of Equation (1) show that the number of moles of gaseous products is far important than the details of the bonding arrangements within the molecular structure. Equation (3) covers the range from the oxygen lean to oxygen rich explosives. The agreement between calculated and measured pressures of the new method is also satisfactory because large percent deviations are generally attributed to experimental measurements of detonation pressure, up to 20 %.

**Glossary** (Compound names for pure as well as composite explosives on the basis of 100 g for mixture of different compounds):

Alex 20:  $\text{C}_{1.783}\text{H}_{2.469}\text{N}_{1.613}\text{O}_{2.039}\text{Al}_{0.7335}$   
 Alex 32:  $\text{C}_{1.647}\text{H}_{2.093}\text{N}_{1.365}\text{O}_{1.744}\text{Al}_{1.142}$   
 BTF: Benzotris[1,2,5]oxadiazole-1,4,7-trioxide ( $\text{C}_6\text{N}_6\text{O}_6$ )  
 COMP B: 63/36/1 RDX/TNT/wax ( $\text{C}_{2.03}\text{H}_{2.64}\text{N}_{2.18}\text{O}_{2.67}$ )  
 COMP B-3: 60/40 RDX/TNT ( $\text{C}_{2.04}\text{H}_{2.50}\text{N}_{2.15}\text{O}_{2.68}$ )  
 CYCLOTOL-78/22: 78/22 RDX/TNT ( $\text{C}_{1.73}\text{H}_{2.59}\text{N}_{2.40}\text{O}_{2.69}$ )  
 CYCLOTOL-77/23: 77/23 RDX/TNT ( $\text{C}_{1.75}\text{H}_{2.59}\text{N}_{2.38}\text{O}_{2.69}$ )  
 CYCLOTOL-75/25: 75/25 RDX/TNT ( $\text{C}_{1.78}\text{H}_{2.58}\text{N}_{2.36}\text{O}_{2.69}$ )  
 CYCLOTOL-65/35: 65/35 RDX/TNT ( $\text{C}_{1.96}\text{H}_{2.53}\text{N}_{2.22}\text{O}_{2.68}$ )  
 CYCLOTOL-50/50: 50/50 RDX/TNT ( $\text{C}_{2.22}\text{H}_{2.45}\text{N}_{2.01}\text{O}_{2.67}$ )  
 DATB: 1,3-Diamino-2,4,6-trinitrobenzene ( $\text{C}_6\text{H}_5\text{N}_5\text{O}_6$ )  
 Destex:  $\text{C}_{2.791}\text{H}_{2.3121}\text{N}_{0.987}\text{O}_{1.975}\text{Al}_{0.6930}$   
 EDC-11: 64/4/30/1/1 HMX/RDX/TNT/wax/trylene  
 ( $\text{C}_{1.986}\text{H}_{2.78}\text{N}_{2.23}\text{O}_{2.63}$ )  
 EDC-24: 95/5 HMX/wax ( $\text{C}_{1.64}\text{H}_{3.29}\text{N}_{2.57}\text{O}_{2.57}$ )  
 FEFO: (1,1-[Methylene bis (oxy)]bis[2-fluoro-2,2-dinitro-ethane]) ( $\text{C}_5\text{H}_6\text{N}_4\text{O}_{10}\text{F}_2$ )  
 HBX-1:  $\text{C}_{2.068}\text{H}_{2.83}\text{N}_{1.586}\text{O}_{2.085}\text{Al}_{0.63}$   
 HMX: Cyclotetramethylenetetranitramine ( $\text{C}_4\text{H}_8\text{N}_8\text{O}_8$ )  
 90.54/9.46 HMX/exon:  $\text{C}_{1.43}\text{H}_{2.61}\text{N}_{2.47}\text{O}_{2.47}\text{F}_{0.15}\text{Cl}_{0.10}$   
 HNAB: 2,2',4,4',6,6'-Hexanitroazobenzene ( $\text{C}_{12}\text{H}_4\text{N}_8\text{O}_{12}$ )  
 Liquid TNT:  $\text{C}_7\text{H}_5\text{N}_3\text{O}_6$   
 LX-04: 85/15HMX/Viton ( $\text{C}_{1.55}\text{H}_{2.58}\text{N}_{2.3}\text{O}_{2.3}\text{F}_{0.52}$ )  
 LX-09: 93/4.6/2.4 HMX/DNPA/FEFO ( $\text{C}_{1.43}\text{H}_{2.74}\text{N}_{2.59}\text{O}_{2.72}\text{F}_{0.02}$ )  
 LX-10: 95/5HMX/Viton A ( $\text{C}_{1.42}\text{H}_{2.66}\text{N}_{2.57}\text{O}_{2.57}\text{F}_{0.17}$ )  
 LX-14: 95.5/4.5 HMX/Estane 5702-F1 ( $\text{C}_{1.52}\text{H}_{2.92}\text{N}_{2.59}\text{O}_{2.66}$ )  
 NG: Nitroglycerine ( $\text{C}_3\text{H}_5\text{N}_3\text{O}_9$ )  
 NM: Nitromethane ( $\text{C}_1\text{H}_3\text{N}_1\text{O}_2$ )  
 60Nitromethane/40UP:  $\text{C}_{1.207}\text{H}_{4.5135}\text{N}_{1.432}\text{O}_{3.309}\text{Cl}_{0.2341}$   
 OCTOL-78/22: 77.6/22.4 HMX/TNT ( $\text{C}_{1.76}\text{H}_{2.58}\text{N}_{2.36}\text{O}_{2.69}$ )

**Table 2.** Comparison between detonation pressures calculated by new and K-J [9] methods for CHNO explosives.

Explosive	$\rho_0 \times 10^{-3}$ [kg m <sup>-3</sup> ]	$P_{Exp}$ [GPa]	$P_{New}$ [GPa]	Dev [%]	$P_{K-J}$ [GPa]	Dev [%]	Explosive	$\rho_0 \times 10^{-3}$ [kg m <sup>-3</sup> ]	$P_{Exp}$ [GPa]	$P_{New}$ [GPa]	Dev [%]	$P_{K-J}$ [GPa]	Dev [%]
HMX	1	11.0 [10]	9.8	-11	10.5	-4	NG	1.6	25.3 [10]	27.0	7	28.6	13
	1.2	16.0 [10]	14.7	-8	15.2	-5	TNM	1.64	15.9 [10]	16.2	2	35.5	124
	1.4	21.0 [10]	20.5	-2	20.7	-2	TATB	1.83	26.0 [10]	23.8	-8	26.1	0
	1.6	28.0 [10]	27.3	-3	27.0	-4		1.85	25.9 [10]	24.4	-6	26.7	3
	1.89	39.0 [10]	38.7	-1	37.7	-3		1.895	31.5 [4]	25.6	-19	28.0	-11
RDX	1.9	39.3 [4]	39.1	-1	38.1	-3	NM	1.13	12.5 [10]	12.5	0	13.0	4
	0.95	9.6 [10]	8.7	-10	9.6	0	FEFO	1.59	25.0 [10]	25.4	1	22.5	-10
	1	8.9 [10]	9.8	10	10.6	19	Cyclotol	1.743	31.3 [4]	31.0	-1	29.6	-6
	1.1	12.2 [10]	12.1	-1	12.8	5	Composition B	1.713	29.4 [4]	28.8	-2	27.4	-7
	1.2	15.2 [10]	14.7	-3	15.3	0	Octol	1.809	34.3 [4]	33.4	-3	32.1	-6
TNT	1.29	16.6 [10]	17.3	4	17.6	6	HNAB	1.6	20.5 [10]	22.6	10	21.3	4
	1.4	21.3 [10]	20.6	-3	20.8	-3	LX-14	1.84	37.0 [10]	35.6	-4	34.4	-7
	1.46	21.1 [10]	22.5	7	22.6	7	PBX-9011	1.77	32.4 [10]	31.2	-4	30.3	-6
	1.6	26.3 [10]	27.3	4	27.1	3	BTF	1.86	36.0 [10]	35.0	-3	31.7	-12
	1.72	31.3 [10]	31.8	2	31.3	0	Cyclotol 50/50 RDX/TNT	1.63	23.1 [10]	24.9	8	24.0	4
	1.77	33.8 [10]	33.8	0	33.2	-2	Cyclotol 65/35 RDX/TNT	1.72	29.2 [10]	29.2	0	28.1	-4
	1.8	34.7 [4]	35.0	1	34.3	-1	Cyclotol 75/25 RDX/TNT	1.76	31.6 [10]	33.0	4	30.4	-4
	0.8	3.7 [10]	3.8	3	4.8	31	Cyclotol 75/25 RDX/TNT	1.62	26.5 [10]	27.7	5	25.7	-3
	1	6.7 [10]	6.8	2	7.6	13	Cyclotol 77/23 RDX/TNT	1.74	31.3 [10]	31.0	-1	29.9	-5
	1.36	12.4 [10]	13.9	12	14.0	13	Cyclotol 78/22 RDX/TNT	1.76	31.7 [10]	31.8	0	30.6	-3
PETN	1.45	14.4 [10]	16.0	11	15.9	11	COMP B-3	1.72	29.5 [10]	28.7	-3	27.6	-7
	1.64	21.0 [10]	20.8	-1	20.4	-3	OCTOL 78/22	1.82	34.2 [10]	34.0	-1	32.7	-4
	0.88	6.8 [10]	7.2	6	8.2	21	OCTOL 76/23	1.81	33.8 [10]	33.5	-1	32.2	-5
	0.99	8.7 [10]	9.5	9	10.4	19	OCTOL 60/40	1.8	32.0 [10]	31.6	-1	30.2	-6
	1.23	13.9 [10]	15.5	11	16.0	15	PENTOLITE 50/50	1.68	25.1 [13]	26.9	7	25.9	3
	1.45	20.8 [10]	22.0	6	22.3	7	PENTOLITE 50/50	1.68	25.1 [13]	26.2	4	25.5	2
	1.6	26.6 [10]	27.2	2	27.1	2	Cyclotol	1.743	31.3 [4]	31.1	-1	29.9	-4
	1.67	30.0 [10]	29.7	-1	29.5	-2	EDC-11	1.782	31.5 [4]	31.2	-1	29.9	-5
	1.7	30.7 [10]	30.9	1	30.6	0	EDC-24	1.776	34.2 [4]	36.3	6	31.7	-7
	1.76	33.7 [10]	33.2	-2	32.8	-3	Liquid TNT	1.447	17.2 [4]	16.0	-7	15.9	-7
Tetryl	1.77	33.5 [4]	33.6	0	33.2	-1	Nitromethane	1.128	14.1 [4]	13.1	-7	13.4	-5
	1.36	14.2 [10]	16.4	16	16.2	14	14.5Toluene/85.5Nitromethane	1.088	10.0 [4]	9.1	-9	10.4	4
	1.61	22.6 [10]	23.6	4	22.7	0	Mean absolute percentage error (MAPE)			4			8
DATB	1.68	23.9 [10]	25.8	8	24.7	3							
	1.78	25.1 [10]	24.2	-4	25.1	0							
	1.788	25.9 [4]	24.4	-6	25.3	-2							
	1.8	25.1 [10]	24.7	-1	25.6	2							

**Table 3.** Comparison between detonation pressures calculated by new method for CHNOFCl explosives.

Explosive	$\rho_0 \times 10^{-3}$ [kg m <sup>-3</sup> ]	$P_{Exp}$ [GPa]	$P_{New}$ [GPa]	Dev [%]	Explosive	$\rho_0 \times 10^{-3}$ [kg m <sup>-3</sup> ]	$P_{Exp}$ [GPa]	$P_{New}$ [GPa]	Dev [%]
FEFO	1.50	25.0 [10]	22.4	-10	65/35 RDX/TFNA	1.754	32.4 [4]	30.6	-6
LX-09	1.84	37.5 [10]	36.1	-4	PBX-9010	1.781	31.9 [4]	32.2	1
LX-04	1.86	35.0 [13]	34.2	-2	90.54/9.46 HMX/Exon	1.833	34.3 [4]	34.7	1
PBX-9407	1.6	28.7 [10]	27.4	-5	PBX-9502	1.894	28.5 [13]	25.0	-12
Lx-10	1.86	37.5 [10]	36.7	-2	90.1/9.1 RDX/Exon	1.786	32.0 [4]	32.4	1
TFNA	1.692	24.9 [4]	24.7	-1					
TFENA	1.523	17.4 [4]	17.0	-2	MAPE				3

OCTOL-76/23: 76.3/23.7 HMX/TNT ( $C_{1.76}H_{2.58}N_{2.37}O_{2.69}$ )  
OCTOL - 60/40: 60/40 HMX/TNT ( $C_{2.04}H_{2.50}N_{2.15}O_{2.68}$ )  
PBX-9010: 90/10 RDX/Kel-F ( $C_{1.39}H_{2.43}N_{2.43}O_{2.43}Cl_{0.09}F_{0.26}$ )  
PBX-9011: 90/10 HMX/Estane ( $C_{1.73}H_{3.18}N_{2.45}O_{2.61}$ )  
PBX-9407: 94/6 RDX/Exon 461 ( $C_{1.41}H_{2.66}N_{2.54}O_{2.54}Cl_{0.07}F_{0.09}$ )  
PBX-9502: 95/5 TATB/ Kel-F 800 ( $C_{2.3}H_{2.23}N_{2.21}O_{2.21}Cl_{0.04}F_{0.13}$ )  
PENTOLITE: 50/50 TNT/ PETN ( $C_{2.33}H_{2.37}N_{1.29}O_{3.22}$ )  
PETN: Pentaerythritoltetranitrate ( $C_5H_8N_4O_{12}$ )

RDX: Cyclomethylenetrinitramine ( $C_3H_6N_6O_6$ )  
RDX/Al(90/10):  $C_{1.215}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$   
RDX/Al(80/20):  $C_{1.081}H_{2.161}N_{2.161}O_{2.161}Al_{0.715}$   
RDX/Al(70/30):  $C_{0.945}H_{1.89}N_{1.89}O_{1.89}Al_{1.11}$   
RDX/Al(60/40):  $C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$   
RDX/Al(50/50):  $C_{0.675}H_{1.35}N_{1.35}O_{1.35}Al_{1.853}$   
65/35 RDX/TFNA:  $C_{1.54}H_{2.64}N_{2.2}O_{2.49}F_{0.44}$   
90.1/9.9 RDX/Exon:  $C_{1.44}H_{2.6}N_{2.44}O_{2.44}F_{0.17}Cl_{0.11}$

**Table 4.** Comparison between pressures calculated by means of the new method for aluminized composite explosives with BKWS-EOS (using full and partial, 50%, interaction of aluminized composite) and measured values.

Explosive	$\rho_0 \times 10^{-3}$ [kg m <sup>-3</sup> ]	$P_{Exp}$ [GPa]	$P_{New}$ [GPa]	Dev [%]	BKWS-EOS, Full [GPa]	Dev [%]	BKWS-EOS, Partial [GPa]	Dev [%]
HBX-1	1.71	22.0 [10]	21.4	−3	—	—	—	—
90RDX/10Al	1.68	24.6 [10]	27.0	10	26.4	7	25.7	4
80RDX/20Al	1.73	22.7 [10]	25.4	12	24.4	7	23.7	4
70RDX/30Al	1.79	21.0 [10]	23.3	11	20.5	−2	21.2	1
60RDX/40Al	1.84	21.1 [10]	20.6	−2	15.6	−26	17.4	−18
50RDX/50Al	1.89	19.0 [10]	17.6	−7	12.0	−37	11.9	−37
TNTEB/Al(90/10)	1.75	26.2 [10]	27.7	6	26.9	3	25.8	−2
TNTEB/Al(80/20)	1.82	24.8 [10]	26.3	6	25.6	3	24.4	−2
TNTEB/Al(70/30)	1.88	22.7 [10]	24.0	6	21.9	−4	21.9	−4
TNT/Al(78.3/21.7)	1.8	18.9 [10]	18.6	−2	18.3	−3	18.7	−1
ALEX20	1.801	23.0 [1]	23.7	3	—	—	—	—
ALEX32	1.88	21.5 [1]	22.8	6	—	—	—	—
Destex	1.68	17.5 [1]	15.0	−15	—	—	—	—
MAPE				7		10		8

TATB: 1,3,5-Triamino-2,4,6-trinitrobenzene (C<sub>6</sub>H<sub>3</sub>N<sub>6</sub>O<sub>6</sub>)

TETRYL: N-Methyl-N-nitro-2,4,6-trinitroaniline (C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O<sub>6</sub>)

TFNA: C<sub>5</sub>H<sub>7</sub>N<sub>4</sub>O<sub>6</sub>F<sub>3</sub>

TFENA: C<sub>2</sub>H<sub>3</sub>N<sub>2</sub>O<sub>2</sub>F<sub>3</sub>

14.5Toluene/85.5Nitromethane: C<sub>2.503</sub>H<sub>5.461</sub>N<sub>1.4006</sub>O<sub>2.8013</sub>

TNETB/Al(90/10): C<sub>1.399</sub>H<sub>1.399</sub>N<sub>1.399</sub>O<sub>3.264</sub>Al<sub>0.371</sub>

TNETB/Al(80/20): C<sub>1.244</sub>H<sub>1.244</sub>N<sub>1.244</sub>O<sub>2.902</sub>Al<sub>0.715</sub>

TNETB/Al(70/30): C<sub>1.088</sub>H<sub>1.088</sub>N<sub>1.088</sub>O<sub>2.539</sub>Al<sub>1.11</sub>

TNT: 2,4,6-Trinitrotoluene (C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>6</sub>)

TNTAB: Trinitrotriazidobenzene (C<sub>6</sub>N<sub>12</sub>O<sub>6</sub>)

TNT/Al(89.4/10.6): C<sub>2.756</sub>H<sub>1.969</sub>N<sub>1.181</sub>O<sub>2.362</sub>Al<sub>0.393</sub>

TNT/Al(78.3/21.7): C<sub>2.414</sub>H<sub>1.724</sub>N<sub>1.034</sub>O<sub>2.069</sub>Al<sub>0.804</sub>

TNT/Al(67.8/32.2): C<sub>2.090</sub>H<sub>1.493</sub>N<sub>1.896</sub>O<sub>1.791</sub>Al<sub>1.193</sub>

## Abbreviations

$\Delta H^0$ (products) – Heats of formation of detonation products [J mol<sup>−1</sup>]

$\Delta H^0$ (c) – Condensed phase heat of formation of the explosive [J mol<sup>−1</sup>]

$Q_{det}$  – Heat of detonation [J kg<sup>−1</sup>]

$P$  – Detonation pressure [GPa]

$n_g$  – Number of moles of gaseous products of detonation per gram of explosive [mol kg<sup>−1</sup>]

$\bar{M}_g$  – Average molecular mass of gaseous products [kg mol<sup>−1</sup>]

$\rho_0$  – Loading density [kg m<sup>−3</sup>]

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