A Simple and Reliable Method for Predicting the Detonation Velocity of CHNOFCl and Aluminized Explosives

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Abstract: A reliable method is introduced for predicting the detonation velocity of CHNOFClAl explosives through suitable decomposition paths. The predicted decomposition products are used to estimate the heat of detonation (decomposition) and the detonation velocity. For non-ideal aluminized explosives, the Chapman-Jouguet detonation velocities are significantly different from those expected from existing thermodynamic computer codes for equilibrium and steady state calculations. The predicted detonation velocities give more reliable results for CHNO explosives than one of the best available empirical methods over a wide range of loading densities. The new model provides better agreement with respect to experimental values for aluminized explosives than the computed results from the BKWS equation of state using full and partial equilibrium of aluminium.

Keywords: decomposition reaction, heat of detonation, detonation velocity, CHNOFClAl explosive, loading density

1 Introduction

The prediction of the detonation properties of new energetic materials should be done prior to their actual synthesis because it reduces the costs associated with synthesis, testing and evaluation of the materials. Due to the difficulties of synthesis and the instability of energetic materials, suitable computer codes or prediction methods can be used to estimate their detonation and propulsion parameters, as well as their thermodynamic and physical properties [1-3]. For the prediction of detonation performance, complex computer codes with an

appropriate empirical equation of state, such as Becker-Kistiakowsky-Wilson (BKW-EOS), or suitable empirical methods can be used.

A detonation wave is a combustion wave propagating at supersonic speeds so that a significant amount of heat is released. According to the Chapman-Jouguet (C-J) theory, the Rayleigh line is tangential to the adiabatic shock of the detonation products at the point, which is assigned as the C-J point. The C-J point corresponds to the end of the chemical reactions. The C-J plane is the surface between the chemical reaction zone and the detonation products [1]. Ideal explosives have a narrow reaction zone and small failure diameters, which are suitable for practical applications. Their performance can be described adequately, for engineering purposes, by steady-state detonation calculations using appropriate equations of state. In contrast to ideal explosives, the physical separation of the fuel and the oxidizer in non-ideal explosives results in an extended chemical reaction zone because diffusion may play a major role in the experimentally determined detonation properties. However, a high degree of inhomogeneity and secondary reactions occurring in the detonation products expanding behind the detonation zone are two important characteristics of non-ideal explosives. In general, non-ideal explosives can have a C-J detonation pressure and velocity significantly different from equilibrium and steady state calculations [4, 5].

Aluminum powder can be incorporated into explosives in order to raise the reaction temperature, enhance the heat of detonation, increase bubble energies in underwater weapons, improve air blast and create an incendiary effect. Aluminized composite explosives show non-ideal behaviour because they have significantly different detonation properties from those predicted by some computer codes, such as CHEETAH [6], which use empirical equations of state. Finely dispersible aluminum powders can also act as intermediate sensitive agents in explosives. For aluminized explosives, combustion of the aluminum particles occurs during the expansion of the gaseous detonation products behind the reaction front. Since aluminum particles do not participate in the reaction zone and act as inert ingredients, thermodynamic calculations of the detonation parameters are carried out by assuming a certain degree of aluminum oxidation.

For non-ideal explosives, as a simple approximation, partial equilibrium rather than a complex reacting mechanism can be used to predict the detonation properties. A certain amount of the initial aluminum is assumed to react in partial equilibrium. Inert aluminum atoms were included in the product species database of computer codes, only in the form of solid, liquid or gaseous aluminum, which prevent aluminum reacting with oxygen or other reactive species. The number of gaseous products can be increased by preventing the aluminum from

forming such products as aluminum oxide. It should be noted that detonation can be improved by increasing the gas yield [1-3]. Aluminum oxide has a large negative heat of formation so that the high-temperature oxidation of aluminum produces a hot, fuel rich gas phase and more solid carbon.
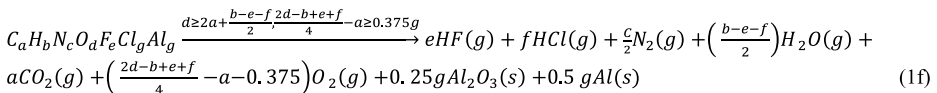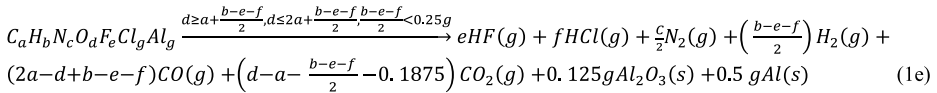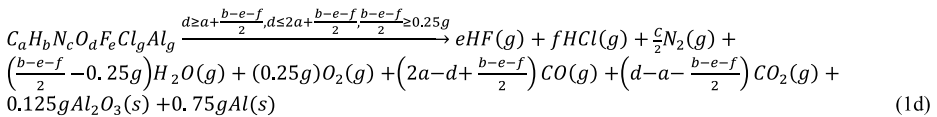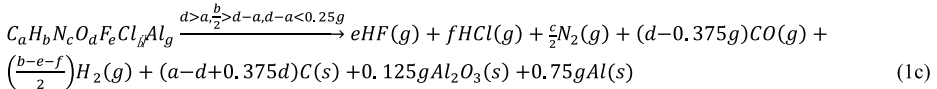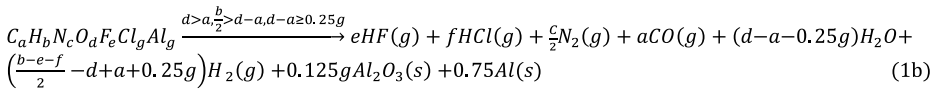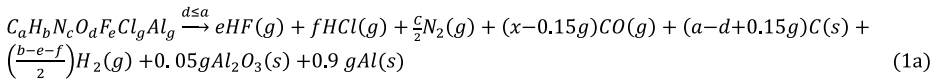
For aluminized explosives, some new methods have been recently introduced to predict the detonation performance of aluminized explosives through the molecular structure of the explosive components [5, 7-12]. For some energetic compounds containing unusual molecular fragments, deviations of these correlations may be large. Moreover, application of these methods to a wide range of ideal and non-ideal explosives is rather limited. The purpose of the present work is to introduce a simple general correlation for calculating the detonation velocity of any explosive with the general formula CHNOFClAl at any loading density. Suitable decomposition paths were selected to specify the detonation products and the detonation velocity for both pure and mixtures of CHNOFCl energetic compounds, as well as aluminized composite explosives. For CHNO explosives, the calculated detonation velocities will also be compared with the Kamlet-Jacobs (K-J) method [13], as well as computed results from the BKWS equation of state using full and partial equilibrium of the aluminum.

2   Materials and Method

Combustion of aluminum particles in aluminized explosives occurs behind the reaction front because aluminum particles do not participate in the reaction zone but act as inert ingredients. However, the detonation parameters can be estimated by assuming a certain degree of aluminum oxidation because its value at the C-J point for a mixture of high explosives with aluminum is not clear. The burning of aluminum particles raises the temperature until it is completely burned near the C-J plane. For aluminized explosives, the amount of reacted aluminum may be a function of the reaction zone length. Since the detonation pressure and velocity increase with a higher gas yield, the high-temperature oxidation of aluminum produces a hot, fuel rich gas phase and more solid carbon. If complete equilibrium is reached, oxygen is forced to react with aluminum rather than carbon, and more condensed aluminum oxide is produced.

Since accurate estimation of the decomposition products from energetic materials remains a major unresolved problem, the equilibrium composition of the products can be determined either through experimental measurement of thermochemical equilibrium or by suggesting appropriate decomposition paths. It was recently found that suitable decomposition reactions can be used

to predict the detonation velocity of various explosives with the general formula $C_aH_bN_cO_dF_eCl_f$, over a wide range of loading densities [5]. For aluminized explosives, the measured detonation velocities are significantly different from those predicted by equilibrium, one dimensional and steady state calculations. Complex thermochemical calculations indicate that 94% of the gaseous products from 34 CHNO explosives consist of CO, H_2O, H_2, N_2 and CO_2 [15]. Previous studies [5, 7-12] have confirmed that the degree of aluminum oxidation depends on the oxygen content of the explosive. According to the participation of aluminum in reaction with the detonation products, it can be assumed that all nitrogen atoms go to N_2, fluorine atoms to HF, and chlorine atoms to HCl, whilst a portion of the oxygen atoms form H_2O, carbon atoms are preferentially oxidized to CO rather than CO_2 and part of the aluminum is oxidized to Al_2O_3. The following pathways can be written to obtain the detonation products on the basis of the oxygen content of the explosive:

$$C_aH_bN_cO_dF_eCl_gAl_g \xrightarrow{d\leq a} eHF(g) + fHCl(g) + \tfrac{c}{2}N_2(g) + (x-0.15g)CO(g) + (a-d+0.15g)C(s) + \left(\tfrac{b-e-f}{2}\right)H_2(g) +0.05gAl_2O_3(s) +0.9\,gAl(s) \tag{1a}$$

$$C_aH_bN_cO_dF_eCl_gAl_g \xrightarrow{d>a,\tfrac{b}{2}>d-a,d-a\geq0.25g} eHF(g) + fHCl(g) + \tfrac{c}{2}N_2(g) + aCO(g) + (d-a-0.25g)H_2O+ \left(\tfrac{b-e-f}{2} -d+a+0.25g\right)H_2(g) +0.125gAl_2O_3(s) +0.75Al(s) \tag{1b}$$

$$C_aH_bN_cO_dF_eCl_fAl_g \xrightarrow{d>a,\tfrac{b}{2}>d-a,d-a<0.25g} eHF(g) + fHCl(g) + \tfrac{c}{2}N_2(g) + (d-0.375g)CO(g) + \left(\tfrac{b-e-f}{2}\right)H_2(g) + (a-d+0.375d)C(s) +0.125gAl_2O_3(s) +0.75gAl(s) \tag{1c}$$

$$C_aH_bN_cO_dF_eCl_gAl_g \xrightarrow{d\geq a+\tfrac{b-e-f}{2},d\leq2a+\tfrac{b-e-f}{2},\tfrac{b-e-f}{2}\geq0.25g} eHF(g) + fHCl(g) + \tfrac{c}{2}N_2(g) + \left(\tfrac{b-e-f}{2} -0.25g\right)H_2O(g) + (0.25g)O_2(g) +\left(2a-d+\tfrac{b-e-f}{2}\right)CO(g) +\left(d-a-\tfrac{b-e-f}{2}\right)CO_2(g) + 0.125gAl_2O_3(s) +0.75gAl(s) \tag{1d}$$

$$C_aH_bN_cO_dF_eCl_gAl_g \xrightarrow{d\geq a+\tfrac{b-e-f}{2},d\leq2a+\tfrac{b-e-f}{2},\tfrac{b-e-f}{2}<0.25g} eHF(g) + fHCl(g) + \tfrac{c}{2}N_2(g) +\left(\tfrac{b-e-f}{2}\right)H_2(g) + (2a-d+b-e-f)CO(g) +\left(d-a-\tfrac{b-e-f}{2}-0.1875\right)CO_2(g) +0.125gAl_2O_3(s) +0.5\,gAl(s) \tag{1e}$$

$$C_aH_bN_cO_dF_eCl_gAl_g \xrightarrow{d\geq2a+\tfrac{b-e-f}{2},\tfrac{2d-b+e+f}{4}-a\geq0.375g} eHF(g) + fHCl(g) + \tfrac{c}{2}N_2(g) +\left(\tfrac{b-e-f}{2}\right)H_2O(g) + aCO_2(g) +\left(\tfrac{2d-b+e+f}{4}-a-0.375\right)O_2(g) +0.25gAl_2O_3(s) +0.5\,gAl(s) \tag{1f}$$

The extent of reaction of aluminum with the decomposition products in the above equations depends on the oxygen balance, which can be estimated on the basis of the measured values of the detonation velocity.

3   Results and Discussion

Organic compounds containing energetic bonds include metastable molecules capable of undergoing very rapid and highly exothermic reactions. The important properties of energetic compounds such as thermal sensitivity and detonation velocity can help in the screening of potential energetic candidates, as well as the selection of only the most promising substances for laboratory synthesis, scale-up, testing *etc*. Studies of the thermolysis and deflagration temperatures of energetic compounds are important parameters for the estimation of their heat sensitivities [16-19]. For some classes of energetic compounds, it was demonstrated that the activation energies of thermal decomposition can be related to their electrostatic sensitivities [16, 17]. However, it is important to have both pure explosives and mixtures of explosives possessing good safety and performance.

From an examination of the detonation velocities of different types of energetic materials, it can be inferred that the detonation velocity depends on three principal parameters:

1) The composition of the energetic material: It is reasonable to assume that all of the chemical bonds present in the reacting molecules are broken, and are subsequently recombined to form stable products. The type and number of moles of gaseous products are two important parameters reflecting the detonation velocity of an explosive as a function of its composition. Some empirical methods have used these parameters for defining and evaluating, in a fairly simple and straightforward manner, the detonation velocity [2, 3].

2) The heat content of the energetic compound: The heat of detonation is another important factor, which depends on the heat of formation, per unit weight, of the explosive is defined as the negative of the enthalpy change of the detonation reaction. It can be determined from the heats of formation of the reactants and the decomposition products of the explosive through the following relation [13]:

$$Q \cong -\frac{\left[\Delta_f H^\theta (detonation\ products) - \Delta_f H^\theta (\text{c})\right]}{formula\ weight\ of\ explosive} \tag{2}$$

where $\Delta_f H^\theta(detonation\ products)$, $\Delta_f H^\theta(\text{c})$ and Q are the heats of formation of the detonation products, the condensed phase heat of formation of the explosive and the heat of detonation, respectively. The heat of detonation is also the most effective parameter for predicting the characteristics of the blast wave pressure and the energy of an underwater explosion. However,

energetic materials possessing a high energy content can release greater energy upon detonation.

3) The loading density: Experimental data of various pure and composite explosives containing aluminum reveals that the detonation velocity may be roughly proportional to the loading density [2, 3, 20].
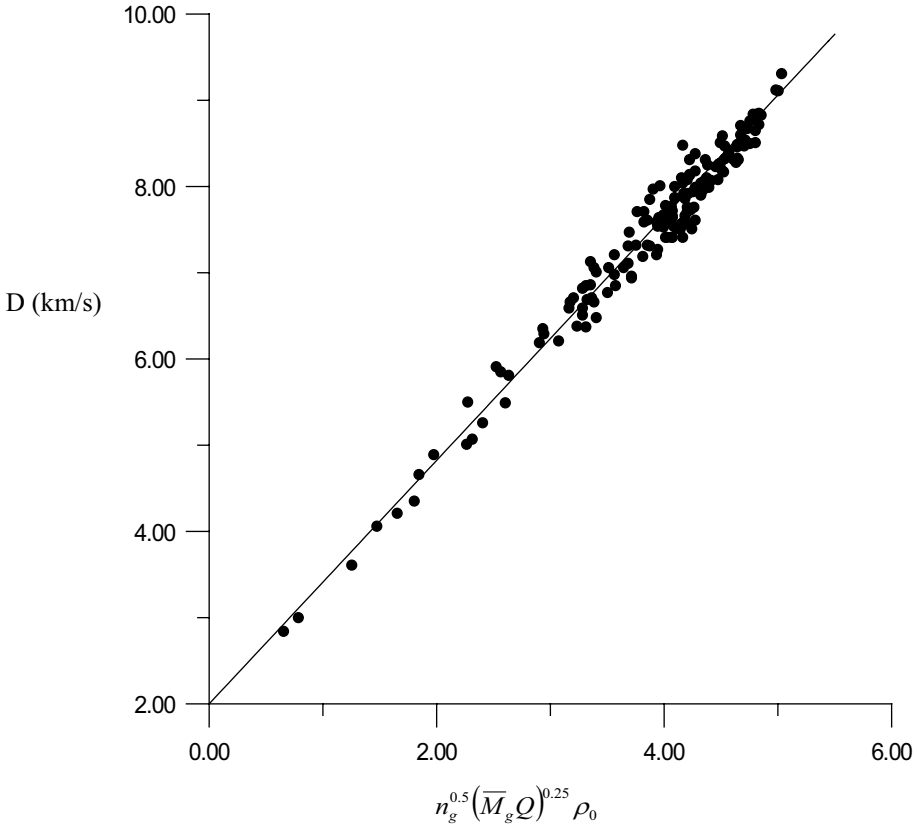
Figure 1. The measured detonation velocity versus $n_g^{0.5}\left(\overline{M}_g Q\right)^{0.25} \rho_0$ for various explosives given in Tables 2-4.

Various combinations of the effective parameters, such as the predicted heats of detonation using Equation (1), the number moles of gaseous products and the loading density have been studied. The necessary parameters for deriving a suitable correlation on the basis of the appropriate decomposition paths of Equation (1) are given in Table 1. The results show that there is a linear

relationship between the measured detonation velocity and $n_g^{0.5}\left(\overline{M}_g Q\right)^{0.25} \rho_0$ for the various explosives given in Tables 2-4. Figure 1 indicates this linear correlation, which can be expressed as the following equation:

$$D = 1.412 n_g^{0.5}\left(\overline{M}_g Q\right)^{0.25} \rho_0 + 2.00 \tag{3}$$

where D is the detonation velocity in km/s, n_g is the number of moles of gaseous products of detonation per gram of explosive, $\overline{M}_g$ is the average molecular weight of the gaseous products and ρ_0 is the loading density. The coefficient of determination (R^2) of Equation (3) was relatively good, being equal to 0.94.

Table 1.   Parameters used in Equation (3)

Explosive	$\Delta_f H^\theta(c)$ [kcal/mol]	Q [cal/g]	n_g [mol/g]	$\overline{M}_g$ [g/mol]
HMX	17.92 [a]	1199	0.0405	24.67
RDX	14.7 [b]	1204	0.0405	24.67
TNT	-16.03 [a]	632	0.0441	21.50
PETN	-128 [b]	1384	0.0348	28.73
Tetryl	4.79 [a]	862	0.0418	23.92
DATB	-23.6 [a]	555	0.0453	22.09
NG	-88.6 [a]	1498	0.0319	31.31
NQ	-22.2 [a]	994	0.0481	20.80
TNM	13 [b]	546	0.0306	32.67
TATB	-33.4 [a]	472	0.0465	21.50
NM	-27.1 [a]	938	0.0492	20.33
FEFO	-177.5 [b]	1258	0.0344	29.09
TFNA	-183.03 [c]	740	0.0435	23.00
TFENA	-166.01 [c]	585	0.0417	24.00
RDX/TFNA (65/35)	-19.04	1018	0.0410	24.36
HMX/Exon (90.54/9.46)	-245.41	1092	0.0409	24.45
RDX/Exon (90.1/9.9)	-46.724	1057	0.0410	24.42
LX-07	-12.3	1049	0.0422	23.71
CYCLOTOL-77/23	-186.011	1038	0.0424	23.61
LX-10	-3.14	1129	0.0414	24.18
COMP B	1	944	0.0434	23.05
TATB/HMX/Kel-F (45/45/10)	-477.99	741	0.0436	22.93
ABH	116 [b]	858	0.0389	25.70

Explosive	$\Delta_f H^\theta(c)$ [kcal/mol]	Q [cal/g]	n_g [mol/g]	$\overline{M}_g$ [g/mol]
DEGN	-99.4 [b]	917	0.0459	21.78
DIPM	-6.8 [b]	683	0.0418	23.89
EXPD	-94 [b]	497	0.0447	22.36
HNAB	67.9 [b]	852	0.0398	25.11
LX-14	1.5	1076	0.0428	23.39
LX-01	-27.5	1210	0.0424	23.58
MEN-II	-74.3	402	0.0625	15.99
NONA	27.4 [b]	792	0.0394	25.40
PBX-9007	7.13	864	0.0480	20.83
PBX-9011	-4.05	925	0.0454	22.00
PBX-9205	-20.8	469	0.0464	21.55
PBX-9501	2.3	1117	0.0420	23.80
PA	-51.3 [b]	721	0.0393	25.44
BTF	144 [b]	1200	0.0357	28.00
HNB	10 [b]	1650	0.0259	38.67
TNTAB	270 [b]	1275	0.0357	28.00
COMP A-3	2.84	875	0.0477	20.95
CYCLOTOL-50/50	0.01	849	0.0445	22.47
CYCLOTOL-60/40	1.33	918	0.0437	22.86
CYCLOTOL-60/40	1.33	918	0.0437	22.86
CYCLOTOL-65/35	1.99	956	0.0433	23.09
CYCLOTOL-70/30	2.66	991	0.0429	23.30
CYCLOTOL-75/25	3.32	1027	0.0464	21.56
CYCLOTOL-75/25	3.32	1117	0.0464	21.56
CYCLOTOL-77/23	3.58	1041	0.0424	23.59
CYCLOTOL-78/22	3.71	1048	0.0423	23.65
COMP C-4	3.33	913	0.0482	20.74
COMP C-3	-6.45	842	0.0448	22.29
COMP B-3	1.33	914	0.0438	22.82
OCTOL-76/23	3.05	1032	0.0424	23.58
OCTOL-75/25	2.89	1022	0.0425	23.52
OCTOL-60/40	0.99	918	0.0437	22.90
PENTOLITE	-19.6	933	0.0416	24.02
LX-09	2	1156	0.0410	24.36
LX-10	2	1156	0.0414	24.18
PBX-9407	0.81	1141	0.0409	24.45

Explosive	$\Delta_f H^\theta(c)$ [kcal/mol]	Q [cal/g]	n_g [mol/g]	$\overline{M}_g$ [g/mol]
PBX-9407	0.81	1197	0.0409	24.45
LX-04	-21.5	964	0.0425	23.54
LX-05	-21.5	964	0.0425	23.54
LX-11	-30.73	890	0.0431	23.21
LX-15	-4.34	679	0.0389	25.67
LX-17	-24.04	470	0.0444	22.48
PBX-9010	-7.87	1087	0.0400	25.03
PBX-9502	-20.8	469	0.0452	22.14
PBX-9503	-17.7	545	0.0452	22.12
HMX/Al (90/10)	5.44	1209	0.0365	24.26
HMX/Al (80/20)	4.83	1220	0.0327	23.78
HMX/Al (70/30)	4.22	1236	0.0284	23.09
HMX/Al (60/40)	3.63	1247	0.0244	22.23
RDX/A (90/10)l	5.95	1214	0.0365	24.26
RDX/Al (80/20)	5.29	1226	0.0327	23.78
RDX/Al (70/30)	4.63	1240	0.0284	22.10
RDX/Al (60/40)	3.97	1249	0.0243	22.22
RDX/Al (50/50)	3.31	1263	0.0203	21.01
TNTEB/Al (90/10)	-27.75	1416	0.0280	31.63
TNTEB/Al (80/20)	-24.66	1405	0.0250	31.01
TNTEB/Al (70/30)	-21.58	1396	0.0218	30.12
TNT/Al (89.4/10.6)	-5.91	630	0.0388	21.40
TNT/Al (78.3/21.7)	-5.17	623	0.0333	21.26
TNT/Al (67.8/32.2)	-4.48	621	0.0281	21.08
Tritonal	-5.65	621	0.0341	21.29
ALEX20	-1.82	817	0.0381	19.56
ALEX32	-2.23	901	0.0306	19.06
PBX C-117	-15.67	735	0.0419	19.19
Destex	-8.22	553	0.0347	19.33
HBX-1	-2.54	778	0.0394	19.39
HBX-3	-2.53	610	0.0311	18.94
PBX-9404	-2.64	1127	0.0394	19.39
PBX-9408	2.31	1130	0.0311	18.94
ONT	0.81	1127	0.0410	24.45
DIPAM	2.31	1130	0.0412	24.24
OCTOL	22.3 [c]	754	0.0390	24.61

Explosive	$\Delta_f H^\theta(c)$ [kcal/mol]	Q [cal/g]	n_g [mol/g]	$\overline{M}_g$ [g/mol]
CYCLOTOL	-3.82 [c]	690	0.0419	23.89
NM/UP (60/40)	-53.71	1048	0.0424	23.60
TFET	3.32	755	0.0424	23.60
PF	-53.71	746	0.0430	23.34
PBXC-9	-137.86 [c]	755	0.0394	25.36
EDC-11	-50.97 [c]	746	0.0390	25.67
EDC-24	27.01	1458	0.0332	23.23
PBXC-116	1.08	907	0.0449	22.24
PBXC-119	4.37	1015	0.0493	22.34
Liquid TNT	-18.24	630	0.0502	19.91
Toluene/Nitromethane (14.5/85.5)	-9.69	887	0.0498	20.07

[*] Experimental values were taken from [a][22], [b][14], and [c][4].

Table 2. Comparison between detonation velocities (in km/s) calculated by the new and the K-J [13] methods for CHNO explosives

Explosive	ρ_0 [g/cm³]	Dexp[*] [km/s]	D_{New} [km/s]	%Dev	D_{K-J} [km/s]	%Dev
HMX	1.9	9.1 [a]	9.08	-0.21	9.12	0.22
	1.89	9.11 [b]	9.04	-0.73	9.09	-0.27
	1.6	7.91 [b]	7.96	0.66	8.09	2.33
	1.4	7.3 [b]	7.22	-1.13	7.41	1.52
	1.2	6.58 [b]	6.47	-1.64	6.73	2.25
	1	5.8 [b]	5.73	-1.27	6.04	4.22
	0.75	4.88 [b]	4.79	-1.74	5.19	6.36
RDX	1.8	8.75 [a]	8.71	-0.40	8.79	0.42
	1.77	8.7 [b]	8.60	-1.12	8.68	-0.19
	1.72	8.46 [b]	8.42	-0.52	8.51	0.62
	1.66	8.24 [b]	8.19	-0.58	8.31	0.82
	1.6	8.13 [b]	7.97	-1.98	8.10	-0.34
	1.46	7.6 [b]	7.45	-2.02	7.62	0.31
	1.4	7.46 [b]	7.22	-3.18	7.42	-0.56
	1.29	7 [b]	6.81	-2.68	7.04	0.60
	1.1	6.18 [b]	6.10	-1.24	6.39	3.44
	0.7	4.65 [b]	4.61	-0.83	5.02	8.05
	0.56	4.05 [b]	4.09	0.96	4.55	12.24

Explosive	ρ_0 [g/cm³]	Dexp* [km/s]	D_{New} [km/s]	%Dev	D_{K-J} [km/s]	%Dev
TNT	1.64	6.95 [b]	7.25	4.32	6.97	0.34
	1.64	6.93 [b]	7.25	4.62	6.97	0.63
	1.45	6.5 [b]	6.64	2.19	6.42	-1.17
	1.36	6.2 [b]	6.35	2.48	6.16	-0.59
	1.061	5.25 [a]	5.40	2.79	5.30	0.91
	1	5 [b]	5.20	4.03	5.12	2.42
	0.8	4.34 [b]	4.56	5.10	4.54	4.66
	0.732	4.2 [b]	4.34	3.42	4.35	3.46
PETN	1.77	8.3 [a]	8.58	3.42	8.69	4.71
	1.76	8.27 [b]	8.55	3.34	8.66	4.67
	1.7	8.07 [b]	8.32	3.14	8.45	4.72
	1.67	7.98 [a]	8.21	2.90	8.35	4.62
	1.6	7.75 [b]	7.95	2.60	8.11	4.63
	1.45	7.18 [b]	7.39	2.97	7.60	5.79
	1.23	6.37 [b]	6.58	3.22	6.84	7.42
	0.99	5.48 [b]	5.68	3.69	6.02	9.87
	0.88	5.06 [b]	5.27	4.21	5.64	11.55
PETN	0.48	3.6 [b]	3.79	5.15	4.28	18.76
	0.3	2.99 [b]	3.12	4.21	3.66	22.39
	0.25	2.83 [a]	2.93	3.53	3.49	23.26
TETRYL	1.73	7.72 [b]	7.98	3.43	7.78	0.74
	1.71	7.85 [b]	7.92	0.83	7.71	-1.72
	1.7	7.56 [a]	7.88	4.24	7.68	1.64
	1.68	7.5 [b]	7.81	4.16	7.62	1.62
	1.61	7.58 [b]	7.57	-0.14	7.40	-2.33
	1.36	6.68 [b]	6.70	0.37	6.63	-0.81
	1.2	6.34 [b]	6.15	-2.98	6.13	-3.35
DATB	1.8	7.6 [b]	7.69	1.21	7.60	0.01
	1.788	7.52 [b]	7.65	1.78	7.57	0.61
NG	1.6	7.7 [b]	7.94	3.09	8.20	6.43
	1.59	7.58 [a]	7.90	4.23	8.18	7.97
NQ	1.78	8.59 b	8.61	0.23	7.87	-8.39
	1.629	7.98 [a]	8.05	0.87	7.40	-7.23
	1.62	7.93 [b]	8.02	1.08	7.38	-6.99
	1.55	7.65 [b]	7.76	1.38	7.16	-6.41
TNM	1.64	6.36 [b]	6.68	5.05	6.67	4.89

Explosive	ρ_0 [g/cm³]	Dexp* [km/s]	D_{New} [km/s]	%Dev	D_{K-J} [km/s]	%Dev
TATB	1.895	7.86 [a]	7.79	-0.88	7.82	-0.45
	1.88	7.76 [b]	7.75	-0.19	7.78	0.27
	1.85	7.66 [b]	7.65	-0.08	7.69	0.43
	1.83	7.58 [b]	7.59	0.17	7.63	0.71
NM	1.13	6.28 [b]	6.16	-1.93	6.38	1.59
COMP B	1.713	8.03 [a]	8.12	1.12	7.98	-0.62
ABH	1.78	7.6 [a]	8.04	5.80	7.69	1.22
	1.64	7.2 [b]	7.57	5.08	7.27	0.98
DEGN	1.38	6.76 [b]	6.96	3.00	7.06	4.38
DIPM	1.76	7.4 [b]	7.74	4.63	7.53	1.70
EXPD	1.55	6.85 [b]	6.75	-1.45	6.80	-0.70
	1.48	6.7 [b]	6.54	-2.44	6.60	-1.54
HNAB	1.6	7.31 [b]	7.45	1.93	7.20	-1.55
LX-14	1.84	8.83 [b]	8.77	-0.68	8.75	-0.95
LX-01	1.24	6.84 [b]	6.69	-2.26	7.12	4.11
MEN-II	1.02	5.49 [b]	5.22	-4.85	5.57	1.53
NONA	1.78	7.56 [a]	7.94	5.05	7.60	0.51
NONA	1.7	7.4 [b]	7.67	3.71	7.36	-0.54
PBX-9007	1.64	8.09 [b]	7.88	-2.64	7.79	-3.73
PBX-9011	1.77	8.5 [b]	8.36	-1.64	8.31	-2.27
PBX-9205	1.67	8.17 [b]	8.05	-1.47	7.98	-2.29
PBX-9501	1.84	8.83 [b]	8.80	-0.35	8.80	-0.30
PA	1.76	7.57 [b]	7.73	2.16	7.55	-0.24
	1.71	7.26 [b]	7.57	4.28	7.40	1.96
	1.6	7.1 [b]	7.21	1.58	7.07	-0.37
BTF	1.86	8.49 [b]	8.72	2.69	8.37	-1.45
	1.76	8.26 [b]	8.36	1.18	8.05	-2.56
HNB	1.97	9.3 [b]	9.11	-1.99	9.19	-1.18
TNTAB	1.74	8.58 [b]	8.38	-2.32	8.25	-3.86
COMP A-3	1.64	8.47 [b]	7.88	-6.91	7.86	-7.16
CYCLOTOL-50/50	1.63	7.66 [b]	7.71	0.60	7.59	-0.92
CYCLOTOL-60/40	1.74	8.09 [b]	8.18	1.13	8.07	-0.27
CYCLOTOL-60/40	1.72	7.9 [b]	8.11	2.67	8.00	1.32
CYCLOTOL-65/35	1.72	8.04 [b]	8.16	1.49	8.07	0.35
CYCLOTOL-70/30	1.73	8.06 [b]	8.24	2.19	8.17	1.30
CYCLOTOL-75/25	1.76	8.3 [b]	8.53	2.77	8.33	0.34

| Explosive	ρ_0 [g/cm³]	Dexp* [km/s]	D_{New} [km/s]	%Dev	D_{K-J} [km/s]	%Dev
CYCLOTOL-75/25	1.62	7.95 [b]	8.14	2.37	7.87	-1.04
CYCLOTOL-77/23	1.74	8.25 [b]	8.33	1.01	8.29	0.46
CYCLOTOL-78/22	1.76	8.31 [b]	8.41	1.24	8.37	0.68
COMP C-4	1.66	8.37 [b]	8.04	-3.98	7.98	-4.71
COMP C-3	1.6	7.63 [b]	7.60	-0.43	7.57	-0.76
COMP B-3	1.72	7.89 [b]	8.11	2.77	8.00	1.34
OCTOL-76/23	1.81	8.45 [b]	8.57	1.45	8.51	0.70
OCTOL-75/25	1.81	8.48 [b]	8.56	0.95	8.49	0.07
OCTOL-60/40	1.8	8.16 [b]	8.40	2.91	8.26	1.18
PENTOLITE	1.71	7.75 [c]	8.03	3.55	7.84	1.20
	1.68	7.65 [c]	7.92	3.53	7.75	1.28
	1.64	7.53 [c]	7.78	3.30	7.62	1.22
DIPAM	1.79	7.5 [a]	7.86	4.83	7.62	1.66
EDC-11	1.782	8.21 [a]	8.35	1.75	8.24	0.32
EDC-24	1.776	8.71 [a]	8.83	1.41	8.49	-2.57
PBXC-116	1.65	7.96 [a]	7.52	-5.47	7.54	-5.28
PBXC-119	1.635	8.07 [a]	7.95	-1.48	7.92	-1.84
Liquid TNT	1.447	6.58 [a]	6.65	1.07	6.43	-2.23
Toluene/Nitromethane (14.5/85.5)	1.088	5.84 [a]	5.62	-3.70	5.79	-0.87
Mean absolute percentage error (MAPE)				2.38		2.96

* Experimental values were taken from [a][4], [b][14], and [c][23].

For CHNO explosives, the calculated detonation velocities of well-known, pure and mixed explosives are given in Table 2. The K-J method [13] is based on an empirical relation, which can be used to predict the detonation velocities of CHNO explosives. It assumes that all of the oxygen available in the explosive is used in the formation of water and carbon dioxide, and none of the oxygen is used in the formation of carbon monoxide. It requires as input only the heats of formation of the explosive and of the simple gas phase products, as well as the loading density. As shown in Table 2, the calculated detonation velocities of explosives using our method are compared with the estimated values from the K-J method [13]. As indicated in Table 2, Equation (2) provides surprisingly very good agreement with experimental data as compared to the K-J method [13]. The calculated detonation velocity for various CHNOFCl are given in Table 3 and compared with those from the K-J method [13], as well as experimental

data. As can be seen, the predicted results are also closer to the experimental values than those from the K-J method [13]. Table 4 contains the predicted detonation velocities for CHNOFClAl explosives, where the calculated results are also compared with computed results from the BKWS-EOS method, using full and partial equilibrium of Al, as well as from the K-J method [13]. For partial equilibrium, only 50% of the aluminum is assumed to interact with the combustion products. As indicated in Table 4, the predicted results of the new method show surprisingly very good agreement with experimental data, compared to the K-J method [13] and the computed results from a complicated computer program for non-ideal aluminized explosives.

The new method has the following advantages with respect to the K-J method:

(i)   The K-J method can be applied only for $C_aH_bN_cO_d$ explosives because it is based on the following decomposition equation [13]:

$$C_aH_bN_cO_d \rightarrow 0.5cN_2 + 0.5bH_2O + (0.5d - 0.25b)CO_2 + (a - 0.5d + 0.25b)C$$

$$(4)$$
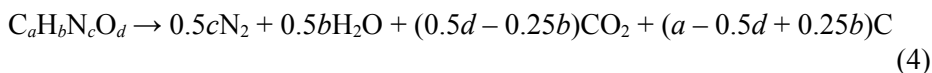
Four decomposition paths and suitable conditions of Equations (2a)-(2d) were assumed for the $C_aH_bN_cO_dF_eCl_fAl_g$ explosives in this study in order to consider ideal $C_aH_bN_cO_d$ explosives as well as halogenated and non-ideal aluminized explosives.

(ii) Although the K-J method can be used for $C_aH_bN_cO_d$ explosives, deviations of the K-J method are high for $C_aH_bN_cO_d$ explosives at loading densities less than 1.0 g/cm³, *e.g.* PETN in Table 2. Equation (3) can give reliable predictions not only for loading densities greater than 1.0 g/cm³, but also for those less than 1.0 g/cm³.

(iii) Since the decomposition path of Equation (4) of the K-J method is valid for $C_aH_bN_cO_d$ explosives, the K-J method may give large deviations for some halogenated explosives [21].

(iv) Since aluminized explosives have non-ideal behaviour, the K-J method cannot be applied for this important class of explosives. However, the four conditions of Equation (2) can assume the extent of reaction of aluminum with the detonation products.

Thus, the new correlation requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical property of the explosive and its detonation products, except for Δ_fH^θ(c) at a specified ρ_0.

Table 3. Comparison between detonation velocities (in km/s) calculated by the new and the K-J [13] methods for CHNOFCl explosives

Explosive	ρ_0 [g/cm^3]	Dexp[*] [km/s]	D_{New} [km/s]	%Dev	D_{K-J} [km/s]	%Dev
FEFO	1.59	7.4 [a]	7.76	4.85	7.40	0.04
TFNA	1.692	7.4 [b]	7.69	3.94	6.39	13.64
TFENA	1.523	6.65 [b]	6.78	1.96	-[**]	-
RDX/TFNA (65/35)	1.754	8.22 [b]	8.29	0.89	8.07	1.81
HMX/Exon (90.54/9.46)	1.833	8.665 [b]	8.69	0.30	8.60	0.76
RDX/Exon (90.1/9.9)	1.786	8.404 [b]	8.47	0.81	7.57	9.88
LX-07	1.865	8.64 [c]	8.79	1.78	8.51	1.52
LX-10	1.86	8.82 [c]	8.87	0.55	8.74	0.92
TATB/HMX/Kel-F (45/45/10)	1.898	8.167 [c]	8.39	2.72	7.91	3.15
LX-09	1.84	8.81 [a]	8.81	0.05	8.83	0.24
LX-10	1.838	8.84 [b]	8.83	-0.14	8.75	1.05
PBX-9407	1.6	7.91 [a]	7.90	-0.07	7.93	0.28
LX-04	1.86	8.46 [c]	8.65	2.19	8.17	3.45
LX-05	1.865	8.53 [b]	8.66	1.56	8.18	4.06
LX-11	1.87	8.32 [c]	8.57	3.03	7.85	5.63
LX-15	1.58	6.84 [c]	7.06	3.16	6.64	2.86
LX-17	1.91	7.63 [c]	7.76	1.72	7.52	1.38
PBX-9010	1.781	8.363 [b]	8.46	1.15	8.34	0.27
PBX-9502	1.9	7.71 [c]	7.76	0.62	7.61	1.27
PBX-9503	1.9	7.72 [c]	7.98	3.32	7.82	1.28
PBX-9404	1.84	8.8 [a]	8.78	-0.25	8.83	0.34
PBX-9404	0.969	5.9 [b]	5.57	-5.60	5.88	0.30
PBX-9408	1.842	8.78 [b]	8.79	0.13	8.83	0.62
NM/UP (60/40)	1.3	6.7 [b]	6.76	0.90	7.13	6.48
TFET	1.786	7.4 [b]	7.89	6.60	6.86	7.24
PF	1.83	7.5 [b]	8.00	6.70	7.36	1.93
Mean absolute percentage error (MAPE)				2.12		2.82

[*] Experimental values were taken from [a][14], [b][4], and [c][23].
[**] Since the predicted heat of detonation of TFENA is negative on the basis of the K-J method, the detonation velocity cannot be calculated.

Table 4. Comparison between the detonation velocities calculated by means of the new method for aluminized composite explosives with BKWS-EOS (using full and partial, 50%, interaction of aluminum with the detonation products), and the K-J [13] method and measured values

Explosive	ρ_0 [g/cm^3]	Dexp* [km/s]	D_{New} [km/s]	%Dev	BKW-EOS, full [km/s]	%Dev	BKW-EOS, partial [km/s]	%Dev	D_{K-J} [km/s]	%Dev
HMX/Al (90/10)	1.76	8.3 [a]	8.21	-1.04	8.32	0.2	8.41	1.3	8.64	4.11
HMX/Al (80/20)	1.82	8.3 [a]	8.06	-2.83	7.93	-4.5	8.22	-1.0	8.85	6.58
HMX/Al (70/30)	1.86	8 [a]	7.75	-3.09	7.27	-9.1	7.82	-2.3	8.98	12.28
HMX/Al (60/40)	1.94	7.7 [a]	7.52	-2.32	6.86	-10.9	7.46	-3.1	8.97	16.54
RDX/Al (90/10)	1.68	8.03 [a]	794	-1.16	8.02	-0.12	8.08	0.6	8.38	4.31
RDX/Al (80/20)	1.73	7.77 [a]	7.77	0.00	7.60	-2.2	7.81	0.5	8.55	9.99
RDX/Al (70/30)	1.79	7.58 [a]	7.54	-0.51	7.03	-7.3	7.49	-1.2	8.75	15.46
RDX/Al (60/40)	1.84	7.2 [a]	7.23	0.38	6.42	-10.8	6.93	-3.8	8.92	23.93
RDX/Al (50/50)	1.89	6.81 [a]	6.85	0.63	5.78	-15.1	6.02	-11.6	9.09	33.54
TNTEB/Al (90/10)	1.75	8.12 [a]	8.02	-1.29	7.85	-3.3	7.91	-2.6	8.49	4.56
TNTEB/Al (80/20)	1.82	7.99 [a]	7.87	-1.50	7.53	-5.8	7.73	-3.3	8.73	9.22
TNTEB/Al (70/30)	1.88	7.84 [a]	7.61	-2.9	6.99	-10.8	7.43	-5.2	8.93	13.89
TNT/Al (89.4/10.6)	1.72	7.05 [a]	7.15	1.49	7.02	-0.4	7.12	1.0	7.21	2.29
TNT/Al (78.3/21.7)	1.8	7.05 [a]	6.98	-1.06	6.59	-6.5	6.94	-1.6	7.44	5.58
TNT/Al (67.8/32.2)	1.89	7.05 [a]	6.79	-3.76	4360	5.94	-15.7	-4.8	7.70	9.27
TriTonal	1.72	6.47 [b]	6.81	5.24	-	-	-	-	7.21	11.38
ALEX20	1.801	7.53 [c]	7.58	0.68	-	-	-	-	8.02	6.46
ALEX32	1.88	7.3 [c]	7.32	0.22	-	-	-	-	8.20	12.31
PBX C-117	1.75	7.7 [c]	7.51	-2.44	-	-	-	-	7.83	1.67
Destex	1.68	6.65 [c]	6.49	-2.36	-	-	-	-	6.77	1.80
PBXC-9	1.975	8.5 [c]	8.89	4.63	-	-	-	-	9.68	13.89
HBX-1	1.71	7.31 [a]	7.31	0.00	-	-	-	-	7.62	4.18
HBX-3	1.84	7.12 [a]	6.75	-5.19	-	-	-	-	7.96	11.78
Mean absolute percentage error (MAPE)				1.94		6.20		2.93		10.22

* Experimental values were taken from [a][14], [b][24], and [c][4].

4   Conclusions

A simple correlation has been introduced for the desk calculation of the detonation velocity of any explosive with general formula $C_aH_bN_cO_dF_eCl_fAl_g$. It requires

only $\Delta_f H^\theta$(c) of the explosive, which can be calculated by suitable methods. For aluminized explosives, the new method does not require using full or partial oxidation of aluminum, which is usually required by a computer code. As shown in Tables 2-4, the agreement between the calculated and measured detonation velocities is satisfactory, because the few percent deviations generally can be attributed to experimental measurements of the detonation velocity.

Acknowledgements

Appendix A.
Glossary of compound names for pure as well as composite explosives on the basis of 100 g for mixtures of different compounds
1. ABH: Azobis(2,2',4,4',6,6'-hexanitrobiphenyl) ($C_{24}H_6N_{14}O_{24}$)
2. Alex 20: $C_{1.783}H_{2.469}N_{1.613}O_{2.039}Al_{0.7335}$
3. Alex 32: $C_{1.647}H_{2.093}N_{1.365}O_{1.744}Al_{1.142}$
4. BTF: Benzotris[1,2,5]oxadiazole-1,4,7-trioxide ($C_6N_6O_6$)
5. COMP B: 63/36/1 RDX/TNT/wax ($C_{2.03}H_{2.64}N_{2.18}O_{2.67}$)
6. COMP A-3 : 91/9 RDX/WAX ($C_{1.87}H_{3.74}N_{2.46}O_{2.46}$)
7. COMP B-3: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
8. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL ($C_{1.90}H_{2.83}N_{2.34}O_{2.60}$)
9. COMP C-4: 91/5.3/2.1/1.6 RDX/TNT/MNT/NC ($C_{1.82}H_{3.54}N_{2.46}O_{2.51}$)
10. CYCLOTOL-78/22: 78/22 RDX/TNT ($C_{1.73}H_{2.59}N_{2.40}O_{2.69}$)
11. CYCLOTOL-77/23: 77/23 RDX/TNT ($C_{1.75}H_{2.59}N_{2.38}O_{2.69}$)
12. CYCLOTOL-75/25: 75/25 RDX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
13. CYCLOTOL-70/30: 70/30 RDX/TNT ($C_{1.87}H_{2.56}N_{2.29}O_{2.68}$)
14. CYCLOTOL-65/35: 65/35 RDX/TNT ($C_{1.96}H_{2.53}N_{2.22}O_{2.68}$)
15. CYCLOTOL-60/40: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
16. CYCLOTOL-50/50: 50/50 RDX/TNT ($C_{2.22}H_{2.45}N_{2.01}O_{2.67}$)
17. DATB: 1,3-Diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
18. DEGN: Diethyleneglycol dinitrate ($C_4H_8N_2O_7$)
19. Destex: $C_{2.791}H_{2.3121}N_{0.987}O_{1.975}Al_{0.6930}$
20. DIPAM: (2.2',4,4',6,6'-Hexanitro-[1,1-biphenyl]-3,3'-diamine) ($C_{12}H_6N_8O_{12}$)
21. DIPM: Dipicramide ($C_{12}H_6N_8O_{12}$)
22. EXP D: Ammonium picrate ($C_6H_6N_4O_7$)
23. EDC-11: 64/4/30/1/1 HMX/RDX/TNT/Wax/Trylene ($C_{1.986}H_{2.78}N_{2.23}O_{2.63}$)

24. EDC-24: 95/5 HMX/Wax ($C_{1.64}H_{3.29}N_{2.57}O_{2.57}$)
25. FEFO: (1,1-[Methylene bis(oxy)]bis[2-fluoro-2,2-dinitroethane]) ($C_5H_6N_4O_{10}F_2$)
26. H-6: $C_{1.888}H_{2.589}N_{1.611}O_{2.00}Al_{0.7415}$
27. HBX-1: $C_{2.068}H_{2.83}N_{1.586}O_{2.085}Al_{0.63}$
28. HBX-3: $C_{1.669}H_{2.1887}N_{1.220}O_{1.603}Al_{1.2977}$
29. HMX: Cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
30. HMX/Al (90/10): $C_{1.216}H_{2.432}N_{2.432}O_{2.432}Al_{0.371}$
31. HMX/Al (80/20): $C_{1.08}H_{2.16}N_{2.16}O_{2.16}Al_{0.715}$
32. HMX/Al (70/30): $C_{0.944}H_{1.888}N_{1.888}O_{1.888}Al_{1.11}$
33. HMX/Al (60/40): $C_{0.812}H_{1.624}N_{1.624}O_{1.624}Al_{1.483}$
34. HMX/Exon (90.54/9.46): $C_{1.43}H_{2.61}N_{2.47}O_{2.47}F_{0.15}Cl_{0.10}$
35. HNAB: 2,2',4,4',6,6'-Hexanitroazobenzene ($C_{12}H_4N_8O_{12}$)
36. HNB: Hexanitrobenzene ($C_6N_6O_{12}$)
37. Liquid TNT: $C_7H_5N_3O_6$
38. LX-01: 51.7/33.2/15.1 NM/TNM/Nitropropane ($C_{1.25}H_{3.73}N_{1.69}O_{3.39}$)
39. LX-05: $C_{1.55}H_{2.58}N_{2.3}O_{2.3}F_{0.53}$
40. LX-07: 90/10 HMX/Viton A ($C_{1.48}H_{2.62}N_{2.43}O_{2.43}F_{0.35}$)
41. LX-09: 93/4.6/2.4 HMX/DNPA/FEFO ($C_{1.43}H_{2.74}N_{2.59}O_{2.72}F_{0.02}$)
42. LX-10: 95/5 HMX/Viton A ($C_{1.42}H_{2.66}N_{2.57}O_{2.57}F_{0.17}$)
43. LX-11: 80/20 HMX/Viton A ($C_{1.61}H_{2.53}N_{2.16}O_{2.16}F_{0.70}$)
44. LX-14: 95.5/4.5 HMX/Estane 5702-F1 ($C_{1.52}H_{2.92}N_{2.59}O_{2.66}$)
45. LX-15: 95/5 HNS-I/Kel-F 800 ($C_{3.05}H_{1.29}N_{1.27}O_{2.53}Cl_{0.04}F_{0.3}$)
46. LX-17: 92.5/7.5 TATB/Kel-F 800 ($C_{2.29}H_{2.18}N_{2.15}O_{2.15}Cl_{0.054}F_{0.2}$)
47. NG: Nitroglycerine ($C_3H_5N_3O_9$)
48. MEN-II: 72.2/23.4/4.4 Nitromethane/Methanol/Ethylenediamine ($C_{2.06}H_{7.06}N_{1.33}O_{3.10}$)
49. NM: Nitromethane ($C_1H_3N_1O_2$)
50. NONA: 2,2',2",4,4',4",6,6',6"-Nonanitroterphenyl ($C_{18}H_5N_9O_{18}$)
51. NQ: Nitroguanidine ($CH_4N_4O_2$)
52. NM/UP (60/40): $C_{1.207}H_{4.5135}N_{1.432}O_{3.309}Cl_{0.2341}$
53. OCTOL-78/22: 77.6/22.4 HMX/TNT ($C_{1.76}H_{2.58}N_{2.36}O_{2.69}$)
54. OCTOL-76/23: 76.3/23.7 HMX/TNT ($C_{1.76}H_{2.58}N_{2.37}O_{2.69}$)
55. OCTOL-75/25: 75/25 HMX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
56. OCTOL-60/40: 60/40 HMX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
57. PBX-9007: 90/9.1/0.5/0.4 RDX/Polystyrene/DOP/Rosin ($C_{1.97}H_{3.22}N_{2.43}O_{2.44}$)
58. PBX-9010: 90/10 RDX/Kel-F ($C_{1.39}H_{2.43}N_{2.43}O_{2.43}Cl_{0.09}F_{0.26}$)
59. PBX-9011: 90/10 HMX/Estane ($C_{1.73}H_{3.18}N_{2.45}O_{2.61}$)
60. PBX-9205: 92/6/2 RDX/Polystyrene/DOP ($C_{1.83}H_{3.14}N_{2.49}O_{2.51}$)

61. PBX-9404: 94/3/3 HMX/NC/CEF ($C_{1.4}H_{2.75}N_{2.57}O_{2.69}Cl_{0.03}P_{0.01}$)
62. PBX-9407: 94/6 RDX/Exon 461 ($C_{1.41}H_{2.66}N_{2.54}O_{2.54}Cl_{0.07}F_{0.09}$)
63. PBX-9408: 94/3.6/2.4 HMX/DNPA/CEF ($C_{1.43}H_{2.78}N_{2.57}O_{2.68}Cl_{0.03}P_{0.01}$)
64. PBX-9501: 95/2.5/2.5 HMX/Estane/BDNPA-F ($C_{1.47}H_{2.86}N_{2.60}O_{2.69}$)
65. PBX-9502: 95/5 TATB/ Kel-F 800 ($C_{2.3}H_{2.23}N_{2.21}O_{2.21}Cl_{0.04}F_{0.13}$)
66. PBX-9503: 15/80/5 HMX/TATB/KEL-F 800 ($C_{2.16}H_{2.28}N_{2.26}O_{2.26}Cl_{0.038}$)
67. PBXC-9: 75/20/5 HMX/Al/Viton ($C_{1.15}H_{2.14}N_{2.03}O_{2.03}F_{0.17}Al_{0.74}$)
68. PBXC-116: 86/14 RDX/Binder ($C_{1.968}H_{3.7463}N_{2.356}O_{2.4744}$)
69. PBXC-117: 71/17/12 RDX/Al/Binder ($C_{1.65}H_{3.1378}N_{1.946}O_{2.048}Al_{0.6303}$)
70. PBXC-119: 82/18 HMX/Binder ($C_{1.817}H_{4.1073}N_{2.2149}O_{2.6880}$)
71. PENTOLITE: 50/50 TNT/ PETN ($C_{2.33}H_{2.37}N_{1.29}O_{3.22}$)
72. PETN: Pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
73. PF: 1-Fluoro-2,4,6-trinitrobenzene ($C_6H_2N_3O_6F$)
74. PA: Picric acid ($C_6H_3N_3O_7$)
75. RDX: Cyclomethylenetrinitramine ($C_3H_6N_6O_6$)
76. RDX/Al (90/10): $C_{1.215}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$
77. RDX/Al (80/20): $C_{1.081}H_{2.161}N_{2.161}O_{2.161}Al_{0.715}$
78. RDX/Al (70/30): $C_{0.945}H_{1.89}N_{1.89}O_{1.89}Al_{1.11}$
79. RDX/Al (60/40): $C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$
80. RDX/Al (50/50): $C_{0.675}H_{1.35}N_{1.35}O_{1.35}Al_{1.853}$
81. RDX/TFNA (65/35): $C_{1.54}H_{2.64}N_{2.2}O_{2.49}F_{0.44}$
82. RDX/Exon (90.1/9.9): $C_{1.44}H_{2.6}N_{2.44}O_{2.44}F_{0.17}Cl_{0.11}$
83. TATB: 1,3,5-Triamino-2,4,6-trinitrobenzene ($C_6H_6N_6O_6$)
84. TATB/HMX/Kel-F(45/45/10): $C_{1.88}H_{2.37}N_{2.26}O_{2.26}F_{0.28}Cl_{0.06}$
85. TETRYL: N-Methyl-N-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
86. TFNA: $C_5H_7N_4O_6F_3$
87. TFENA: $C_2H_3N_2O_2F_3$
88. TFET: 2,4,6-Trinitrophenyl-2,2,2-trifluoroethylnitramine ($C_8H_4N_5O_8F_3$)
89. Toluene/Nitromethane (14.5/85.5): $C_{2.503}H_{5.461}N_{1.4006}O_{2.8013}$
90. TNETB/Al (90/10): $C_{1.399}H_{1.399}N_{1.399}O_{3.264}Al_{0.371}$
91. TNETB/Al (80/20): $C_{1.244}H_{1.244}N_{1.244}O_{2.902}Al_{0.715}$
92. TNETB/Al (70/30): $C_{1.088}H_{1.088}N_{1.088}O_{2.539}Al_{1.11}$
93. TNM: Tetranitromethane (CN_4O_8)
94. TNT: 2,4,6-Trinitrotoluene ($C_7H_5N_3O_6$)
95. TNTAB: Trinitrotriazidobenzene ($C_6N_{12}O_6$)
96. TNT/Al (89.4/10.6): $C_{2.756}H_{1.969}N_{1.181}O_{2.362}Al_{0.393}$
97. TNT/Al (78.3/21.7): $C_{2.414}H_{1.724}N_{1.034}O_{2.069}Al_{0.804}$
98. TNT/Al (67.8/32.2): $C_{2.090}H_{1.493}N_{1.896}O_{1.791}Al_{1.193}$
99. Tritonal: $C_{2.465}H_{1.76}N_{1.06}O_{2.11}Al_{0.741}$

5   References

[1]   Agrawal J.P., *High Energy Materials: Propellants, Explosives and Pyrotechnics*, WILEY-VCH, Weinheim, **2010**.

[2]   Sikder A.K., Maddala G., Agrawal J.P., Singh H., Important Aspects of Behaviour of Organic Energetic Compounds: A Review, *J. Hazard. Mater. A*, **2001**, *84*, 1-26.

[3]   Keshavarz M.H., Research Progress on Heats of Formation and Detonation of Energetic Compounds, in: *Hazardous Materials: Types, Risks and Control*, (Brar S.K., Ed.), Nova Science Publishers Inc., New York, **2011**, pp. 339-359.

[4]   Mader C.L., *Numerical Modelling of Explosives and Propellants*, 3rd ed., CRC Press, Boca Raton, **2008**.

[5]   Keshavarz M.H., Predicting Detonation Performance in Non-ideal Explosives by Empirical Methods, in: Explosive Materials: Classification, Composition and Properties, (Janssen T.J., Ed.), Nova Science Publishers, New York, **2011**, pp. 179-201.

[6]   Fried L.E., Howard W.M., Souers P.C., *CHEETAH 2.0 User's Manual*, Lawrence Livermore National Laboratory, Livermore, **1998**.

[7]   Keshavarz M.H., New Method for Predicting Detonation Velocities of Aluminized Explosives, *Combust. Flame*, **2005**, *142*, 303-307.

[8]   Keshavarz M.H., Teimuri Mofrad R., Esmail Poor K., Shokrollahi A., Zali A., Yousefi M.H., Determination of Performance of Non-ideal Aluminized Explosives, *J. Hazard. Mater. A*, **2006**, *137*, 83-87.

[9]   Keshavarz M.H., Simple Correlation for Predicting Detonation Velocity of Ideal and Non-ideal Explosives, *J. Hazard. Mater.*, **2009**, *166*, 762-769.

[10] Keshavarz M.H., Prediction of Detonation Performance of CHNO and CHNOAl Explosives through Molecular Structure, *J. Hazard. Mater.*, **2009**, *166*, 1296-1301.

[11] Keshavarz M.H., Shokrolahi A., Pouretedal H.R., A New Method to Predict Maximum Attainable Detonation Pressure of Ideal and Aluminized Energetic Compounds, *High Temp-High Press.*, **2012**, *41*, 349-365.

[12] Keshavarz M.H., Predicting Maximum Attainable Detonation Velocity of CHNOF and Aluminized Explosives, *Propellants Explos. Pyrotech.*, **2012**, *37*, 489-497.

[13] Kamlet M.J., Jacobs S.J., Chemistry of Detonations. I. A Simple Method for Calculating Detonation Properties of C-H-N-O Explosives, *J. Chem. Phys.*, **1968**, *48*, 23-35.

[14] Hobbs M.L., Baer M.R., Calibrating the BKW-EOS with a Large Product Species Database and Measured C-J Properties, *Tenth Symposium (Int.) on Detonation*, Boston, **1993**.

[15] Rice B.M., Hare J., Predicting Heats of Detonation Using Quantum Mechanical Calculations, *Thermochim. Acta*, **2002**, *384*, 377-391.

[16] Keshavarz M.H., Zohari N., Seyedsadjadi S.A., Relationship between Electric Spark Sensitivity and Activation Energy of the Thermal Decomposition of Nitramines for Safety Measures in Industrial Processes, *J. Loss Prev. Process Indust.*, **2013**, *26*, 1452-1456.

[17] Zohari N., Keshavarz M.H., Seyedsadjadi S.A., A Novel Method for Risk Assessment of Electrostatic Sensitivity of Nitroaromatics through Their Activation Energies of Thermal Decomposition, *J. Therm. Anal. Calorim.*, **2014**, *115*, 93-100.

[18] Keshavarz M.H., Zohari N., Seyedsadjadi S.A., Validation of Improved Simple Method for Prediction of Activation Energy of the Thermal Decomposition of Energetic Compounds, *J. Therm. Anal. Calorim.*, **2013**, *114*, 497-510.

[19] Keshavarz M.H., Moradi S., Ebrahimi Saatluo B., Rahimi H., Madram A., A Simple Accurate Model for Prediction of Deflagration Temperature of Energetic Compounds, *J. Therm. Anal. Calorim*., **2013**, *112*, 1453-1463.

[20] Politzer P., Murray, J.S., Some Perspectives on Estimating Detonation Properties of C, H, N, O Compounds, *Cent. Eur. J. Energ. Mater.*, **2011**, *8*, 209-220.

[21] Keshavarz M.H., Pouretedal H.R., Estimation of Detonation Velocity of CHNOFCl Explosives, *High Temp-High Press*, **2003/2006**, *35/36*, 593-600.

[22] Meyer R., Köhler J., Homburg A., *Explosives*, 6th ed., WILEY-VCH, Weinheim, **2007**.

[23] Dobratz B.M., Crawford P.C., *LLNL Explosives Handbook Properties of Chemical Explosives and Explosive Stimulants*, Lawrence Livermore National Labroratory, California, **1985**.

[24] Lu J.P., *Evaluation of the Thermochemical Code CHEETAH 2.0 for Modelling Explosives Performance*, DSTO-TR-1199, **2001**.