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Software Development for the Detonation Product Analysis of High Energetic Materials - Part I

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Abstract: The detonation of energetic materials will result in the formation of decomposition products. These may be carbon monoxide, carbon dioxide, carbon, water, etc. In order to clarify the problems of decomposition products, a software package is developed to solve the problems of decomposition products using four different concepts. Although each concept will provide a different answer for the decomposition products they can be used as a guide and give fairly good approximations. This paper describes the development of a software package to estimate the possible decomposition products and the results generated using the software package LION. An algorithm to compute the detonation products of energetic materials using four different concepts along with the computation of oxygen balance, elemental composition, and molecular weight has been developed and described in this paper. The concept or predicting possible detonation products is particularly useful as one of the guideline for screening the potential molecules, when formulating explosives to produce a minimum toxic fumes to reduce the toxic hazardous to the users.

Keywords: detonation products, explosives, energetic materials, volume of detonation products, oxygen balance, software

Introduction

High energetic materials (HEMs) are unique for having a strong exothermic reactivity, which has made them desirable for both military and commercial applications. These explosives are one of the more difficult classes of organic compounds to identify and characterize in a systematic way. Approaches to this, include conventional chemical methods and analytical methods. However,

the conventional method through time tested, reliable and producing accurate results, requires large infrastructure, large quantity of reagents, solvents and glass wares. They are time consuming and are not eco-friendly [1]. The detonation decomposition products and oxygen balance will be useful in designing better explosive compositions [2].

Information regarding high energetic material properties is necessary for efficiently building the next generation of explosives as the quest for more powerful energetic materials (in terms of energy per volume) moves forward [3-18]. In addition, predicting the detonation products has important ramifications in disposing of such materials safely and cheaply, as there exists vast stockpiles of HEMs with corresponding contamination of earth and groundwater at these sites [4].

For the existing computer codes such as BKW code [19-22], TIGER code [23, 24], VLW code [25, 26], the user has to give molecular weight, density, heat of formation and many complex thermodynamic parameters as input parameter. Also these software's requires huge constants such as coefficients of EOS - α, β, θ, κ; coefficients for Entropy fit - A, B, C, D, F, Enthalpy integration constant - IC, Heat of formation (Elements at 0K to Species at 0K) co-volume, etc. Also the number of coefficients different when different type of EOS is used. It is also observed that for the same EOS like BKW EOS, coefficients of EOS - α, β, θ, κ have been adjusted to different extent by different researchers [27-31]. Apart from the huge input constants, the user has to input some guess values for P, V, T to start the iteration as well as initial guess of the concentrations of the products. Some time the iteration will not converge due to improper wrong initial guess values. In case of using JWL EOS, the accuracy of the computation depends upon the selection (or assumption) of six independent variables A, B, R_1, R_2, C, ω (ω varies between 0.25 to 0.75). While using different EOS, the user needs more mathematical background and knowledge about different coefficients. Whereas LION as described in the work is totally independent of variables and coefficients. Hence it is highly user-friendly.

In the present work, the molecular weight is computed in-suit in the programme itself. Also, it simultaneously computes the detonation products by four different concepts. Hence the user can get an insight of possible detonation product compositions based on four concepts without any complex input parameters. In addition to the computation of detonation products, volume of detonation products, oxygen balance and molecular weight; LION computes the percentage composition of individual elements of given molecule and this result will be handy for the synthetic chemists to verify their experimental elemental analysis results.

Methodology

The detonation of energetic materials will result in the formation of its decomposition products. These may be carbon monoxide, carbon dioxide, carbon, water, etc. In order to clarify the problems of decomposition products set of rules was developed by various researchers and briefly discussed in this section. Although each rule will provide a different answer for the decomposition products they can be used as a guide and give fairly good approximations.

Kistiakowsky-Wilson Concept

In the problem of decomposition products, a set of rules was developed during World War II by Kistiakowsky and Wilson. These rules are nowadays known as the 'Kistiakowsky-Wilson' rules (K-W rules). These rules should only be used for moderately oxygen deficient explosives with an oxygen balance greater than – 40.0.

The Kistiakowsky-Wilson concept rules are presented in Table 1.

Table 1. Kistiakowsky-Wilson rules

Priority No.	Priority conditions
1	Carbon atoms are converted to carbon monoxide $C + O \rightarrow CO$
2	If any oxygen remains then hydrogen is oxidized to water $2H + O \rightarrow H_2O$
3	If any oxygen still remains then carbon monoxide is oxidized to carbon dioxide $CO + O \rightarrow CO_2$
4	All the nitrogen is converted to nitrogen gas, N_2

Modified Kistiakowsky-Wilson Concept

The Kistiakowsky-Wilson concept cannot be used for explosive materials which have an oxygen balance lower than – 40. Under these circumstances the modified Kistiakowsky-Wilson concept has to be employed. The modified Kistiakowsky-Wilson rules are given in Table 2.

Table 2. Modified Kistiakowsky-Wilson rules

Priority No.	Priority conditions
1	Hydrogen atoms are converted to water
2	If any oxygen remains then carbon is converted to carbon monoxide
3	If any oxygen still remains then carbon monoxide is oxidized to carbon dioxide $CO + O \rightarrow CO_2$
4	All the nitrogen is converted to nitrogen gas, N_2

Springall-Roberts Concept

A variation to Kistiakowsky-Wilson and modified Kistiakowsky-Wilson rules is provided by the Springall-Roberts rules. The Springall-Robert rules take the unmodified Kistiakowsky-Wilson rules and add on two more conditions as shown in Table 3.

Table 3. Springall-Roberts rules

Priority No.	Priority conditions
1	Carbon atoms are converted to carbon monoxide $C + O \rightarrow CO$
2	If any oxygen remains then hydrogen is oxidized to water $2H + O \rightarrow H_2O$
3	If any oxygen still remains then carbon monoxide is oxidized to carbon dioxide $CO + O \rightarrow CO_2$
4	All the nitrogen is converted to nitrogen gas, N_2
5	One third of the carbon monoxide formed is converted to carbon and carbon dioxide
6	One sixth of the original amount of carbon monoxide is converted to form carbon and water

Keshavarz Concept

Keshavarz et al. proposed [32] an approximation that all nitrogens go to N_2, fluorines to HF, chlorines to HCl, while a portion of the oxygens form H_2O and carbons preferentially will be oxidized to CO rather than CO_2. The following pathways can be written to obtain detonation products of an energetic materials having composition $C_aH_bN_cO_dF_eCl_f$:

Case 1: $d \le a$

$$eHF + fHCl + \frac{c}{2}N_2 + dCO + (a - d)C_s + \left(\frac{b-e-f}{2}\right)H_2$$

Case 2: $d > a$ and $\left(\frac{b-e-f}{2}\right) > d\text{-}a$

$$eHF + fHCl + \frac{c}{2}N_2 + aCO + (d - a)H_2O + \left(\frac{b-e-f}{2} - d + a\right)H_2$$

Case 3: $d \ge a + \left(\frac{b-e-f}{2}\right)$ and $d \le 2a + \left(\frac{b-e-f}{2}\right)$

$$eHF + fHCl + \frac{c}{2}N_2 + \left(\frac{b-e-f}{2}\right)H_2O + \left(2a - d + \frac{b-e-f}{2}\right)CO + \left(d - a - \frac{b-e-f}{2}\right)CO_2$$

Case 4: $d > 2a + \left(\frac{b-e-f}{2}\right)$

$$eHF + fHCl + \frac{c}{2}N_2 + \left(\frac{b-e-f}{2}\right)H_2O + aCO_2 + \left(\frac{2d-b+e+f}{4} - a\right)O_2$$

Volume of detonation products

The volume of gas produced during a detonation will provide information on the amount of work done by the explosive. In order to measure the volume of gas generated standard conditions must be established, because the volume of gas will vary according to the temperature at which the measurement is taken. These standard conditions also enable comparisons to be made between one explosive and another. The standard conditions set the temperature at 0 °C or 273 K, and the pressure at 1 atm. These conditions are known as 'standard temperature and pressure', 'stp'. Under these standard conditions one mole of gas will occupy 22.4 dm^3, which is known as the molar gas volume. The volume of gas V produced from an explosive during detonation can be calculated from its equation of decomposition, where information can be obtained on the amount of gaseous products liberated.

Oxygen Balance

"Oxygen balance" is one of the method of quantifying how well an explosive provides its own oxidant [33]. Most of the energy released comes from oxidation (reaction with oxygen), the amount of oxygen available is a critical factor. The relative amount of oxygen with respect to the oxygen required to oxidize

the fuel completely in an explosive (or propellant) is expressed quantitatively as 'oxygen balance" [34]. Oxygen balance expresses the number of oxygen molecules remaining after oxidation of C, H, Al, F, Cl, to produce H_2O, CO, Al_2O_3, etc. If excess oxygen molecules are remaining after the oxidation reaction, the oxidizer is said to have a 'positive' oxygen balance. If the oxygen molecules are completely consumed and excess fuel molecules remain, the oxidizer is said to have a 'negative' oxygen balance [35].

It is observed that the heat of detonation reaches a maximum for an oxygen balance of zero, since this corresponds to the stoichiometric oxidation of carbon to carbon dioxide, hydrogen to water and all of its metal to metal oxide with no excess, the molecule is said to have a zero oxygen balance. The oxygen balance can therefore be used to optimize the composition of the explosive to give an oxygen balance as close to zero as possible.

One area in which oxygen balance can be applied is in the processing of mixtures of explosives. The family of explosives called 'amatols' are mixtures of ammonium nitrate and TNT. Ammonium nitrate has an oxygen balance of +20% and TNT has an oxygen balance of −74%, so it would appear that the mixture yielding an oxygen balance of zero would also result in the best explosive properties. In actual practice a mixture of 80% ammonium nitrate and 20% TNT by weight yields an oxygen balance of +1%, the best properties of all mixtures, and an increase in strength of 30% over TNT. Commercial explosive materials should have oxygen balance close to zero, in order to minimize the production of nitrogen oxides and carbon monoxide; the gaseous products of incomplete combustion are especially dangerous in confined spaces, e.g. coal mines.

For an explosive which contains only some or all of the atoms: aluminium, boron, carbon, calcium, chlorine, fluorine, hydrogen, potassium, nitrogen, sodium and oxygen (with the formula Al_{al}, B_b, C_c, Ca_{ca}, Cl_{cl}, F_f, H_h, K_k, N_n, Na_{na}, O_o), the oxygen balance will be

$$OB = -\frac{32\left(\frac{3}{4}al + \frac{3}{4}b + 1c + \frac{1}{2}ca - \frac{1}{4}cl - \frac{1}{4}f + \frac{1}{4}h + \frac{1}{4}k + 0n + \frac{1}{4}na - \frac{1}{2}o\right)}{\textit{explosive molecular weight}} \; x \;\; 100,$$

where the indices al, b, ca, cl, f, h, k, n, na and o, denote the number of atoms of each element in a mole of the explosive composition. The contribution of nitrogen to the oxygen balance is zero since it does not bind to the other elements. It is assumed that there is enough hydrogen in the formulation to bind chlorine and fluorine to hydrochloric and hydrofluoric acids.

Results and Discussion

Accurate determination of product decomposition species for energetic materials with complex elemental composition remains a major unresolved problem. Explosives for use underground, mines, tunnel constructions and other commercial applications with poor ventilation should be formulated to produce a minimum total toxic effect. If there are not enough oxygen atoms in energetic materials for carbon dioxide to be formed then toxic gases such as carbon monoxide will be liberated. This is very important for commercial explosives, as the amount of toxic gases liberated must be kept to a minimum. The concept of predicting possible detonation products is particularly useful as one of the guideline when formulating explosives to produce a minimum toxic fumes to reduce the toxic hazardous to the users.

The detonation products and volume of gaseous products computed using LION by Kistiakowsky-Wilson concept, modified Kistiakowsky-Wilson concept and Keshavarz concept are tabulated in Table 5, 6 and 7 respectively and the results are comparable to the reported in literature [2, 32]. In addition to the computation of detonation products, volume of gaseous products, LION computes the percentage composition of input molecule and this result will be handy for the synthetic chemists to verify their experimental elemental analysis results and some of the results are tabulated in Table 8 and 9. The algorithm utilized in the programming of LION is presented as a schematic flow chart in Figure 2.

Generally, complex thermochemical computer codes are based on different EOS such as BKW, JWL, etc. For solving these EOS, we need to have some initial guesses on detonation products, so that the algorithm in these complex thermochemical computer codes will converge to give more precise theoretical detonation products. If the initial guesses on detonation products are not appropriate, then it may lead to non convergence in solving EOS by the thermo chemical computer codes. Therefore appropriate initial smart guesses on detonation products are important to start the iterative computation algorithm for more precise theoretical detonation products by complex thermochemical computer codes. The algorithm on detonation products computation presented in this article will also be useful to start the iterative computation algorithm to solve the complex thermochemical EOS, so that the iterative algorithm will converge efficiently and the details about algorithm on solving complex thermochemical EOS will be discussed as part – II, which considers the experimental conditions such as density.

Table 5. Detonation products and volume of gas products computed using LION based on K-W rules

Sr No.	Explosive Substance	Computed using LION	
		Detonation (decomposition) products based on K-W rules	Volume of gas products (dm^3/mol)
1	Nitroglycerine	$C_3H_5N_3O_9 \rightarrow 3CO_2 + 2.5H_2O + 1.5N_2 + 0.5O_2$	168
2	EGDN	$C_2H_4N_2O_6 \rightarrow 2CO_2 + 2H_2O + N_2$	112
3	PETN	$C_5H_8N_4O_{12} \rightarrow 3CO_2 + 2CO + 4H_2O + 2N_2$	246.4
4	RDX	$C_3H_6N_6O_6 \rightarrow 3CO + 3H_2O + 3N_2$	201.6
5	HMX	$C_4H_8N_8O_8 \rightarrow 4CO + 4H_2O + 4N_2$	268.8
6	Nitroguanidine	$CH_4N_4O_2 \rightarrow CO + H_2O + H_2 + 2N_2$	112

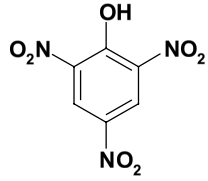
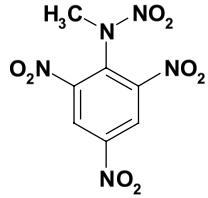
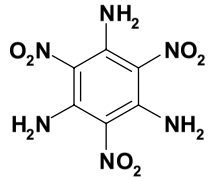
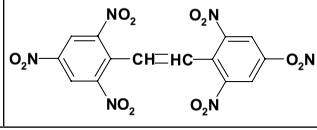
Table 6. Detonation products and volume of gas products computed using LION based on modified K-W rules

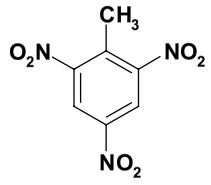
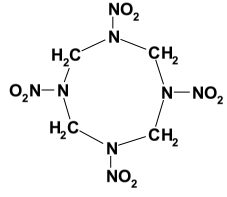
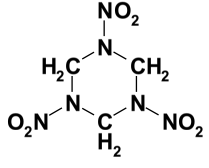
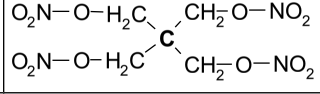
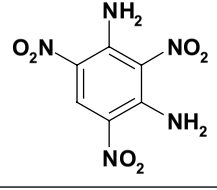
Sr No.	Explosive Substance	Computed using LION	
		Detonation (decomposition) products based on modified K-W rules	Volume of gas products (dm^3/mol)
1	Picric acid	$C_6H_3N_3O_7 \rightarrow 5.5CO + 1.5H_2O + 1.5N_2 + 0.5C$	190.4
2	Tetryl	$C_6H_5N_5O_8 \rightarrow 5.5CO + 2.5H_2O + 2.5N_2 + 0.5C$	235.2
3	TATB	$C_6H_6N_6O_6 \rightarrow 3CO + 3H_2O + 3N_2 + 3C$	201.6
4	HNS	$C_{14}H_6N_6O_{12} \rightarrow 9CO + 3H_2O + 3N_2 + 5C$	336
5	TNT	$C_7H_5N_3O_6 \rightarrow 3.5CO + 2.5H_2O + 1.5N_2 + 3.5C$	168

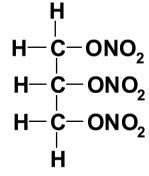
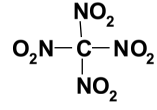
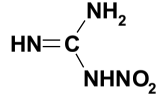
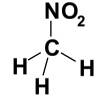
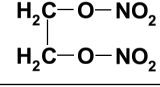
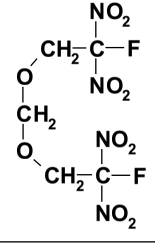
Table 7. Detonation products and volume of gas products computed using LION based on Keshavarz concept

Sr No.	Explosive substance	Computed using LION	
		Detonation (decomposition) products based on modified Keshavarz concept	Volume of gas products (dm^3/mol)
1	HMX	$C_4H_8N_8O_8 \rightarrow 4N_2 + 4CO + 4H_2O$	268.8
2	RDX	$C_3H_6N_6O_6 \rightarrow 3N_2 + 3CO + 3H_2O$	201.6
3	TNT	$C_7H_5N_3O_6 \rightarrow 1.5N_2 + 6CO + C + 2.5H_2$	246.4
4	NQ	$CH_4N_4O_2 \rightarrow 2N_2 + CO + H_2O + H_2$	112.0
5	TETRYL	$C_6H_5N_5O_8 \rightarrow 2.5N_2 + 6CO + 2H_2O + 0.5H_2$	246.4
6	NM	$CH_3NO_2 \rightarrow 0.5N_2 + CO + H_2O + 0.5H_2$	67.2
7	NG	$C_3H_5N_3O_9 \rightarrow 1.5N_2 + 3CO_2 + 2.5H_2O + 0.25O_2$	162.4
8	TNM	$CN_4O_8 \rightarrow 2N_2 + CO_2 + 3O_2$	134.4
9	PETN	$C_5H_8N_4O_{12} \rightarrow 2N_2 + 2CO + 3CO_2 + 4H_2O$	246.4
10	TATB	$C_6H_6N_6O_6 \rightarrow 3N_2 + 6CO + 3H_2$	268.8
11	DATB	$C_6H_5N_5O_6 \rightarrow 2.5N_2 + 6CO + 2.5H_2$	246.4
12	FEFO	$C_5F_2H_6N_4O_{10} \rightarrow 2HF + 2N_2 + 2CO + 3CO_2 + 2H_2O$	246.4
13	TFNA	$C_5F_3H_7N_4O_6 \rightarrow 3HF + 2N_2 + 5CO + H_2O + H_2$	268.8
14	TFENA	$C_2F_3H_3N_2O_2 \rightarrow 3HF + N_2 + 2CO$	134.4
15	Composition B	$C_{6.851}H_{8.75}N_{7.65}O_{9.3} \rightarrow 3.825N_2 + 6.851CO + 2.449H_2O + 1.926H_2$	337.1
16	Cyclotol	$C_{5.045}H_{7.461}N_{6.876}O_{7.753} \rightarrow 3.438N_2 + 5.045CO + 2.708H_2O + 1.0225H_2$	273.6
17	Octol	$C_{6.835}H_{10.025}N_{9.215}O_{10.43} \rightarrow 4.6075N_2 + 6.835CO + 3.595H_2O + 1.4175H_2$	368.5
18	PBX – 9010	$C_{3.42}H_6N_6O_6F_{0.6354}Cl_{0.212} \rightarrow 0.6354HF + 0.212HCl + 3N_2 + 3.4163CO + 3.69978E\text{-}03CO_2 + 2.5763H_2O$	220.5
19	PBX – 9502	$C_{6.27}H_{6.085}N_6O_6F_{0.3662}Cl_{0.123} \rightarrow 0.3662HF + 0.123HCl + 3N_2 + 6CO + 0.27C + 2.7979H_2$	281.3

Table 8. Percentage composition and molecular weight computed using LION

Sr No.	Explosive substance	Molecular formula	Structure	Computed using LION					
				Composition analysis				Molecular weight	Oxygen balance
				C	H	N	O		
1	Picric acid	$C_6H_3N_3O_7$		31.454	1.320	18.344	48.882	229.1199	-45.3911
2	Tetryl	$C_6H_5N_5O_8$		26.1910	1.8316	25.4583	46.5191	275.1558	-37.7967
3	TATB	$C_6H_6N_6O_6$		27.9138	2.3425	32.5594	37.1843	258.1738	-55.7764
4	HNS	$C_{14}H_6N_6O_{12}$		37.3458	1.3432	18.6691	42.6419	450.2618	-67.5163

5	TNT	$C_7H_5N_3O_6$		37.0144	2.2188	18.5034	42.2634	227.1468	-73.9609
6	HMX	$C_4H_8N_8O_8$		16.2208	2.7225	37.8409	43.2158	296.1877	-21.6079
7	RDX	$C_3H_6N_6O_6$		16.2208	2.7225	37.8409	43.2158	222.1408	-21.6079
8	PETN	$C_5H_8N_4O_{12}$		18.9952	2.5505	17.7253	60.7290	316.1587	-10.1215
9	DATB	$C_6H_5N_5O_6$		29.6378	2.0727	28.8087	39.4808	243.1558	-55.9312

10	NG	$C_3H_5N_3O_9$		15.8664	2.2192	18.5070	63.4074	227.1028	3.5226
11	TNM	CN_4O_8		6.1265	0	28.5844	65.2891	196.0510	48.9668
12	NQ	$CH_4N_4O_2$		11.5399	3.8737	53.8417	30.7447	104.0829	-30.7447
13	NM	CH_3NO_2		19.6757	4.9536	22.9503	52.4204	61.0449	-39.3153
14	EGDN	$C_2H_4N_2O_6$		15.7963	2.6513	18.4252	63.1272	152.0738	0
15	FEFO	$C_5F_2H_6N_4O_{10}$		18.7588	1.8891	17.5047	49.9777 F= 11.8697	320.1428	-9.9955

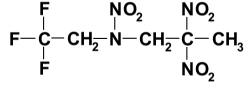
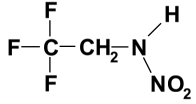
16	TFNA	$C_5F_3H_7N_4O_6$		21.7472	2.5550	20.2933	34.7636 F= 20.6409	276.1507	-34.7636
17	TFENA	$C_2F_3H_3N_2O_2$		16.6743	2.0990	19.4494	22.2121 F= 39.5652	144.0659	-22.2120

Table 9. Percentage composition computed using LION for mixed explosive compositions

Sr No.	Name of the composition	Molecular formula	Ingredients	Computed using LION					
				Composition analysis				Molecular weight	Oxygen balance
				C	H	N	O		
1	Composition B	$C_{6.851}H_{8.75}N_{7.65}O_{9.3}$	64% RDX 36% TNT	23.7082	2.5411	30.8791	42.8715	347.0836	-40.4605
2	Cyclotol	$C_{5.045}H_{7.461}N_{6.876}O_{7.753}$	77% RDX 23% TNT	21.0039	2.6068	33.3913	42.998	288.4967	-33.6503
3	Octol	$C_{6.835}H_{10.025}N_{9.215}O_{10.43}$	76.3% HMX 23.7% TNT	21.1486	2.6032	33.2581	42.9901	388.1822	-34.0149
4	PBX – 9010	$C_{3.42}H_6N_6O_6F_{0.6354}Cl_{0.212}$	90% RDX 10% Kel–F	16.6458	2.4508	34.0635	38.9020 F= 4.8922 Cl= 3.0457	246.7741	-22.1501
5	PBX – 9502	$C_{6.27}H_{6.085}N_6O_6F_{0.3662}Cl_{0.123}$	95% TATB 5% Kel–F	27.6038	2.2482	30.8114	35.1879 F= 2.5503 Cl= 1.5984	272.8209	-54.7635

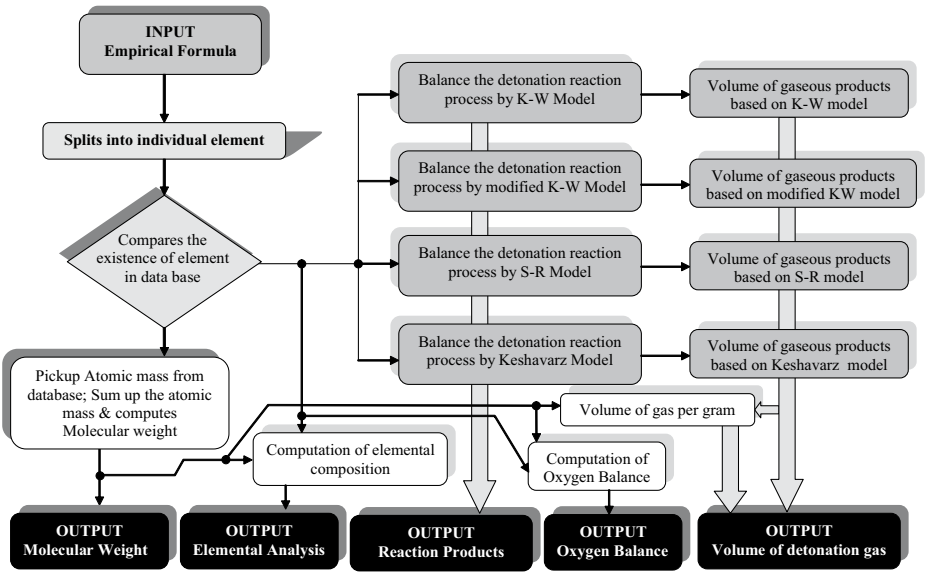


Figure 2. Schematic flow chart of algorithm utilized in the programming of LION.

Conclusion

An algorithm to compute the detonation products of energetic materials using four different concepts along with the computation of oxygen balance, elemental composition, and molecular weight has been developed without complex thermodynamic input parameters. The computer code – LION has been validated with well-known explosives and their compositions. The new algorithm to compute the detonation products of energetic materials is particularly useful as one of the guideline when formulating explosives or compositions to produce minimum toxic gases to reduce the toxic or hazardous side-effects on the users. This allows theoretical screening of notional materials for identification the promising energetic materials and compositions to produce minimum toxic gases for additional study and elimination of weaker candidates from further consideration, thereby reducing cost associated with the development programme of the high energy materials. Also the algorithm on detonation products computation presented in this article will be useful to start the iterative computation algorithm to solve the complex thermochemical EOS, so that the iterative algorithm will converge efficiently.

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