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Computer code for the optimization of performance parameters of mixed explosive formulations

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Abstract

LOTUSES is a novel computer code, which has been developed for the prediction of various thermodynamic properties such as heat of formation, heat of explosion, volume of explosion gaseous products and other related performance parameters. In this paper, we report LOTUSES (Version 1.4) code which has been utilized for the optimization of various high explosives in different combinations to obtain maximum possible velocity of detonation. LOTUSES (Version 1.4) code will vary the composition of mixed explosives automatically in the range of 1–100% and computes the oxygen balance as well as the velocity of detonation for various compositions in preset steps. Further, the code suggests the compositions for which least oxygen balance and the higher velocity of detonation could be achieved. Presently, the code can be applied for two component explosive compositions. The code has been validated with well-known explosives like, TNT, HNS, HNF, TATB, RDX, HMX, AN, DNA, CL-20 and TNAZ in different combinations. The new algorithm incorporated in LOTUSES (Version 1.4) enhances the efficiency and makes it a more powerful tool for the scientists/researches working in the field of high energy materials/hazardous materials.
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Keywords: Mixed explosives; Velocity of detonation; Oxygen balance; Explosive formulations; Modelling; Hazardous materials

1. Introduction

The study of energetic systems by theoretical methods has accelerated dramatically over the course of the last two decades and has proved considerable insight into the understanding of energetic materials [1–5]. The ability to predict the performance parameters of new explosive formulation is very much useful before one undertakes the laborious and expensive process of synthesising/formulating the same. Rigorous theoretical and mathematical approaches developed at present allow us to formalize the knowledge of specialists in formulation of mixed explosive composition. Most explosive and propellant compositions contain a mixture of components to have a maximum performance. Some of the components may not contribute to the heat liberated and may not even contain oxygen. These materials may however, contribute to the gaseous products and reduce the actual temperatures obtained on detonation of the explosive or burning of the propellant. For example, the explosive amatol contains 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%, and shows an increase in strength of 30% over TNT.

Computation to get maximum performance properties of mixed explosive composition by repeated iteration calls for tedious calculation. A new algorithm developed by authors is time saving as well as accurate for the prediction of performance parameters of mixed explosive composition and it is successfully incorporated with LOTUSES code. LOTUSES also can predict the velocity of detonation, density, C–J pressure, heat of explosion, heat of formation, volume of explosion of gaseous products, etc. [6–10]. The new algorithm incorporated enhances its efficiency and allow theoretical screening of notional hazardous materials for identification of promising mixed explosive composition for additional study and elimination of weaker can-

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didates from further consideration. Thereby, reduces the cost associated with the development programme of the high energy materials as well as reduces the duration of development programme. In this paper, we report the velocity of detonation and oxygen balance of mixed explosive formulations computed by LOTUSES (Version 1.4) at different compositions in brief.

Thermochemical/hydrodynamic computer codes such as BKW (Charles L. Mader, first in 1956 for IBM 704, STRETCH BKW in 1961 for IBM 7030, using Fortran IV BKW in 1967) [11–14], RUBY [15], TIGER [16,17], PANDA [18], CHEQ code [19], and CHEETAH [20] have been reported in literature for the prediction of various thermodynamic as well as detonation parameters. But these codes does not gives automatically the optimum composition corresponds to maximum detonation velocity and minimum oxygen balance of mixed explosive formulations. Hence, a new algorithm incorporated in LOTUSES-1.4, which automatically varies the composition of mixed explosive formulations and gives the optimum composition corresponds to maximum detonation velocity and minimum oxygen balance will be of immense value for the scientists, academicians and technologists working in the field of HEMs for designing high performance mixed explosive formulations.

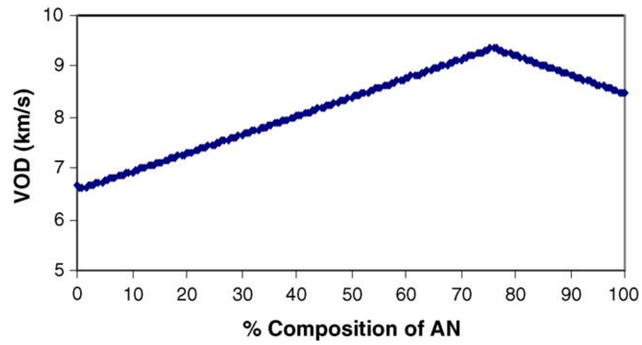


Fig. 1. VOD vs. % composition of AN with TNT.

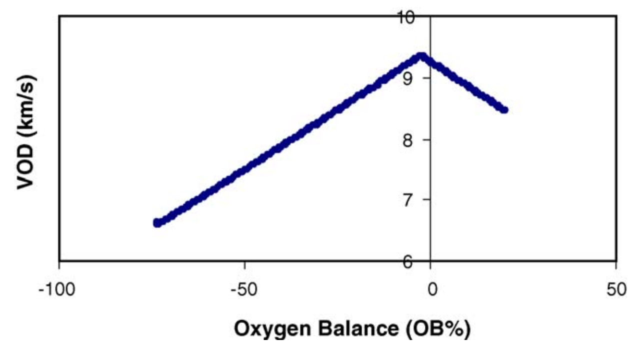


Fig. 2. VOD vs. OB of AN with TNT.

2. Computation of HEMs parameter

2.1. Evaluating oxygen balance

Oxygen balance (OB) of an explosive is a highly important parameter to decide its performance and is defined as the percentage excess/deficiency of oxygen in the explosive molecule to completely oxidize carbon, hydrogen to CO_2 and H_2O, respectively. It is observed that the heat of explosion reaches a maximum for an oxygen balance of zero, since this corresponds to the stoichiometric oxidation of carbon to carbon dioxide and hydrogen to water. 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 [21,22].

The oxygen balance provides information about the types of gases liberated during explosion. If the oxygen balance is large and negative then there is not enough oxygen for carbon dioxide to be formed. Consequently, 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. Explosives for use underground with poor ventilation should be formulated to produce a minimum total toxic effect. The molecule is said to have a positive oxygen balance if it contains more oxygen than is needed. An explosive with excess oxygen produces toxic NO and NO_2. Commercial explosives are usually close to oxygen-balanced, so that the main detonation products are water, carbon dioxide, and nitrogen. The sensitivity, strength and brisance of an explosive are all somewhat dependent upon oxygen balance and tend to approach their maximum as oxygen balance approaches zero. The limitation of OB it that, OB does not provide information on the energy changes which take place during an explosion.

The oxygen balance (OB) is calculated from the empirical formula of a compound in percentage of oxygen required for complete conversion of carbon to carbon dioxide, hydrogen to water and metal to metal oxide. The procedure for calculating oxygen balance in terms of 100 g of the explosive material is to determine the number of gram atoms of oxygen that are excess or deficient for 100 g of a compound. A quantitative measure of oxygen balance can be defined as

$$\mathrm{OB} = \frac{-100 \times \mathrm{MW(O)} \times [2\mathrm{C} + \mathrm{H}/2 + \mathrm{M{-}O}]}{\mathrm{MW(explosive)}}$$

where C, H, M and O are the number of carbon, hydrogen, metal and oxygen in a molecule, MW(O) is the molecular weight of oxygen (=16 g/mol) and MW(explosive) is the molecular weight of explosive.

2.2. Velocity of detonation

Velocity of detonation (VOD) is the rate of propagation of the explosive reaction through the explosive material [23]. Detonation is a form of reaction given by an explosive substance in which the chemical reaction produces a shock wave. High temperature and pressure gradients are generated in the wave front, so that the chemical reaction is initiated instantaneously. Knowledge of the detonation velocity is important because it is the easiest of the C–J state parameters to measure accurately and used to determine all of the other C–J state parameters [24]. A number of attempts have been made over the last few decades to theoretically predict the VOD of explosives [25–36]. In the present work, we have used the Rothstein et al. method [25,26] for the computation of velocity of detonation of mixed explosive composition to get the maximum performance.

Table 1
Velocity of detonation (VOD) and oxygen balance (OB) of mixed explosive composition predicted by LOTUSES Version 1.4

S. no.	Compound	Molecular formula	Computation by LOTUSES 1.4			
			%	Mixed composition	OB (%)	VOD (km/s)
1	RDX	$C_3H_6N_6O_6$	90	$C_{1.52361}H_{2.65101}N_{2.56296}O_{2.69503}$	−26.84	8.799
	TNT	$C_7H_5N_3O_6$	10			
2	RDX	$C_3H_6N_6O_6$	80	$C_{1.6967}H_{2.60103}N_{2.4249}O_{2.68908}$	−32.0	8.552
	TNT	$C_7H_5N_3O_6$	20			
3	RDX	$C_3H_6N_6O_6$	70	$C_{1.8698}H_{2.55105}N_{2.2869}O_{2.68313}$	−37.31	8.305
	TNT	$C_7H_5N_3O_6$	30			
4	HMX	$C_4H_8N_8O_8$	90	$C_{1.52361}H_{2.65101}N_{2.56296}O_{2.69503}$	−26.84	8.799
	TNT	$C_7H_5N_3O_6$	10			
5	HMX	$C_4H_8N_8O_8$	80	$C_{1.69673}H_{2.60103}N_{2.42493}O_{2.68908}$	−32.07	8.552
	TNT	$C_7H_5N_3O_6$	20			
6	HMX	$C_4H_8N_8O_8$	70	$C_{1.86985}H_{2.55105}N_{2.28691}O_{2.68313}$	−37.31	8.305
	TNT	$C_7H_5N_3O_6$	30			
7	ONC	$C_8N_8O_{16}$	90	$C_{1.85933}H_{.26662}N_{1.68323}O_{3.36647}$	−7.76	9.238
	TNT	$C_7H_5N_3O_6$	10			
8	ONC	$C_8N_8O_{16}$	80	$C_{1.99515}H_{.52663}N_{1.64295}O_{3.28591}$	−15.46	8.941
	TNT	$C_7H_5N_3O_6$	20			
9	ONC	$C_8N_8O_{16}$	70	$C_{2.13097}H_{.77335}N_{1.60267}O_{3.20535}$	−23.06	8.645
	TNT	$C_7H_5N_3O_6$	30			
10	TATB	$C_6H_6N_6O_6$	90	$C_{2.09161}H_{2.5912}N_{2.34145}O_{2.46637}$	−48.20	7.919
	AN	$H_4N_2O_3$	10			
11	TATB	$C_6H_6N_6O_6$	80	$C_{1.85921}H_{2.85856}N_{2.35888}O_{2.6087}$	−40.62	8.169
	AN	$H_4N_2O_3$	20			
12	TATB	$C_6H_6N_6O_6$	70	$C_{1.6268}H_{3.12583}N_{2.37632}O_{2.75108}$	−33.04	8.422
	AN	$H_4N_2O_3$	30			
13	TNT	$C_7H_5N_3O_6$	90	$C_{2.77353}H_{2.4807}N_{1.43849}O_{2.75207}$	−64.56	6.933
	AN	$H_4N_2O_3$	10			
14	TNT	$C_7H_5N_3O_6$	80	$C_{2.46536}H_{2.7603}N_{1.5562}O_{2.8626}$	−55.17	7.291
	AN	$H_4N_2O_3$	20			
15	TNT	$C_7H_5N_3O_6$	70	$C_{2.1571}H_{3.0398}N_{1.67402}O_{2.97329}$	−45.77	7.653
	AN	$H_4N_2O_3$	30			
16	HNS	$C_{14}H_6N_6O_{12}$	90	$C_{2.79837}H_{1.69897}N_{1.44914}O_{2.77336}$	−58.76	7.253
	AN	$H_4N_2O_3$	10			
17	HNS	$C_{14}H_6N_6O_{12}$	80	$C_{2.48744}H_{2.06539}N_{1.5657}O_{2.8816}$	−50.01	7.567
	AN	$H_4N_2O_3$	20			
18	HNS	$C_{14}H_6N_6O_{12}$	70	$C_{2.17651}H_{2.43181}N_{1.6823}O_{2.98985}$	−41.26	7.888
	AN	$H_4N_2O_3$	30			
19	CL-20	$C_6H_6N_{12}O_{12}$	90	$C_{1.5403}H_{1.45234}N_{2.59651}O_{2.72858}$	−17.25	9.331
	TNT	$C_7H_5N_3O_6$	10			
20	CL-20	$C_6H_6N_{12}O_{12}$	80	$C_{1.71164}H_{1.5355}N_{2.45475}O_{2.7189}$	−23.55	9.026
	TNT	$C_7H_5N_3O_6$	20			
21	CL-20	$C_6H_6N_{12}O_{12}$	70	$C_{1.8829}H_{1.61875}N_{2.313}O_{2.70922}$	−29.85	8.721
	TNT	$C_7H_5N_3O_6$	30			
22	CL-20	$C_6H_6N_{12}O_{12}$	90	$C_{1.38838}H_{1.44043}N_{2.67265}O_{2.77676}$	−11.52	8.963
	TNAZ	$C_3H_4N_4O_6$	10			
23	CL-20	$C_6H_6N_{12}O_{12}$	80	$C_{1.40763}H_{1.51174}N_{2.60705}O_{2.8152}$	−12.09	8.897
	TNAZ	$C_3H_4N_4O_6$	20			
24	CL-20	$C_6H_6N_{12}O_{12}$	70	$C_{1.42688}H_{1.58305}N_{2.54144}O_{2.85377}$	−12.66	8.832
	TNAZ	$C_3H_4N_4O_6$	30			
25	TEX	$C_6H_6N_4O_8$	90	$C_{2.21602}H_{2.26807}N_{1.58145}O_{3.058809}$	−40.11	7.896
	TNAZ	$C_3H_4N_4O_6$	10			
26	TEX	$C_6H_6N_4O_8$	80	$C_{2.14331}H_{2.24742}N_{1.63709}O_{3.06597}$	−37.50	8.017
	TNAZ	$C_3H_4N_4O_6$	20			
27	TEX	$C_6H_6N_4O_8$	70	$C_{2.070607}H_{2.226772}N_{1.69273}O_{3.073139}$	−34.90	8.139
	TNAZ	$C_3H_4N_4O_6$	30			
28	TEX	$C_6H_6N_4O_8$	90	$C_{2.36803}H_{2.27998}N_{1.50531}O_{3.01062}$	−45.84	7.655
	TNT	$C_7H_5N_3O_6$	10			
29	TEX	$C_6H_6N_4O_8$	80	$C_{2.44732}H_{2.2712}N_{1.4848}O_{2.969608}$	−48.97	7.536
	TNT	$C_7H_5N_3O_6$	20			
30	TEX	$C_6H_6N_4O_8$	70	$C_{2.52662}H_{2.26247}N_{1.46429}O_{2.9285}$	−52.09	7.418
	TNT	$C_7H_5N_3O_6$	30			
31	ONC	$C_8N_8O_{16}$	90	$C_{1.90443}H_{.36678}N_{1.65209}O_{3.35466}$	−10.19	9.130
	DNA	$C_7H_6N_2O_5$	10			

Table 1 (*Continued*)

S. no.	Compound	Molecular formula	Computation by LOTUSES 1.4			
			%	Mixed composition	OB (%)	VOD (km/s)
32	ONC	$C_8N_8O_{16}$	80	$C_{2.08536}H_{.72446}N_{1.58068}O_{3.26230}$	−20.30	8.725
	DNA	$C_7H_6N_2O_5$	20			
33	ONC	$C_8N_8O_{16}$	70	$C_{2.26629}H_{1.06386}N_{1.50926}O_{3.1699}$	−30.26	8.322
	DNA	$C_7H_6N_2O_5$	30			
34	CL-20	$C_6H_6N_{12}O_{12}$	90	$C_{1.58549}H_{1.53502}N_{2.56537}O_{2.71677}$	−19.54	9.22
	DNA	$C_7H_6N_2O_5$	10			
35	CL-20	$C_6H_6N_{12}O_{12}$	80	$C_{2.01822}H_{1.86681}N_{2.21959}O_{2.67380}$	−28.14	8.810
	DNA	$C_7H_6N_2O_5$	20			
36	CL-20	$C_6H_6N_{12}O_{12}$	70	$C_{1.8018}H_{1.70092}N_{2.39248}O_{2.69529}$	−36.73	8.395
	DNA	$C_7H_6N_2O_5$	30			
37	TATB	$C_6H_6N_6O_6$	90	$C_{2.4448}H_{2.39442}N_{2.1925}O_{2.34395}$	−59.88	7.452
	DNA	$C_7H_6N_2O_5$	10			
38	TATB	$C_6H_6N_6O_6$	80	$C_{2.56576}H_{2.4648}N_{2.06108}O_{2.36389}$	−64.00	7.230
	DNA	$C_7H_6N_2O_5$	20			
39	TATB	$C_6H_6N_6O_6$	70	$C_{2.68664}H_{2.5352}N_{1.9296}O_{2.38383}$	−68.11	7.009
	DNA	$C_7H_6N_2O_5$	30			
40	HMX	$C_4H_8N_8O_8$	90	$C_{1.56872}H_{2.73369}N_{2.5318}O_{2.68323}$	−29.13	8.689
	DNA	$C_7H_6N_2O_5$	10			
41	HMX	$C_4H_8N_8O_8$	80	$C_{1.7869}H_{2.7664}N_{2.3626}O_{2.66547}$	−36.66	8.331
	DNA	$C_7H_6N_2O_5$	20			
42	HMX	$C_4H_8N_8O_8$	70	$C_{2.00517}H_{2.79911}N_{2.193502}O_{2.64771}$	−44.19	7.974
	DNA	$C_7H_6N_2O_5$	30			
43	RDX	$C_3H_6N_6O_6$	90	$C_{1.56872}H_{2.73369}N_{2.53182}O_{2.68323}$	−29.13	8.689
	DNA	$C_7H_6N_2O_5$	10			
44	RDX	$C_3H_6N_6O_6$	80	$C_{1.7869}H_{2.766409}N_{2.36266}O_{2.66547}$	−36.66	8.331
	DNA	$C_7H_6N_2O_5$	20			
45	RDX	$C_3H_6N_6O_6$	70	$C_{2.00517}H_{2.799119}N_{2.193501}O_{2.64771}$	−44.19	7.974
	DNA	$C_7H_6N_2O_5$	30			
46	ONC	$C_8N_8O_{16}$	90	$C_{1.70732}H_{.25221}N_{1.75938}O_{3.41465}$	−2.01	9.469
	TNAZ	$C_3H_4N_4O_6$	10			
47	ONC	$C_8N_8O_{16}$	80	$C_{1.69114}H_{.498159}N_{1.79525}O_{3.38228}$	−3.98	9.404
	TNAZ	$C_3H_4N_4O_6$	20			
48	ONC	$C_8N_8O_{16}$	70	$C_{1.67495}H_{.73154}N_{1.83111}O_{3.3499}$	−5.84	9.344
	TNAZ	$C_3H_4N_4O_6$	30			
49	HNS	$C_{14}H_6N_6O_{12}$	90	$C_{2.95453}H_{1.40752}N_{1.40752}O_{2.710934}$	−62.43	7.149
	TNAZ	$C_3H_4N_4O_6$	10			
50	HNS	$C_{14}H_6N_6O_{12}$	80	$C_{2.79977}H_{1.48248}N_{1.482486}O_{2.756751}$	−57.34	7.352
	TNAZ	$C_3H_4N_4O_6$	20			
51	HNS	$C_{14}H_6N_6O_{12}$	70	$C_{2.645005}H_{1.557449}N_{1.5574}O_{2.80256}$	−52.25	7.555
	TNAZ	$C_3H_4N_4O_6$	30			
52	TATB	$C_6H_6N_6O_6$	90	$C_{2.247779}H_{2.29983}N_{2.29983}O_{2.40394}$	−51.86	7.815
	TNAZ	$C_3H_4N_4O_6$	10			
53	TATB	$C_6H_6N_6O_6$	80	$C_{2.17154}H_{2.27565}N_{2.27565}O_{2.48387}$	−47.95	7.954
	TNAZ	$C_3H_4N_4O_6$	20			
54	TATB	$C_6H_6N_6O_6$	70	$C_{2.095305}H_{2.25147}N_{2.25147}O_{2.56379}$	−44.04	8.090
	TNAZ	$C_3H_4N_4O_6$	30			
55	FOX-7	$C_2H_4N_4O_4$	90	$C_{1.523616}H_{2.65101}N_{2.56296}O_{2.69503}$	−26.84	8.799
	TNT	$C_7H_5N_3O_6$	10			
56	FOX-7	$C_2H_4N_4O_4$	80	$C_{1.69673}H_{2.60103}N_{2.42493}O_{2.68908}$	−32.07	8.552
	TNT	$C_7H_5N_3O_6$	20			
57	FOX-7	$C_2H_4N_4O_4$	70	$C_{1.869858}H_{2.55105}N_{2.28691}O_{2.68313}$	−37.31	8.305
	TNT	$C_7H_5N_3O_6$	30			
58	FOX-7	$C_2H_4N_4O_4$	90	$C_{1.56872}H_{2.73369}N_{2.53182}O_{2.68323}$	−29.13	8.689
	DNA	$C_7H_6N_2O_5$	10			
59	FOX-7	$C_2H_4N_4O_4$	80	$C_{1.7869}H_{2.7664}N_{2.362664}O_{2.66547}$	−36.66	8.331
	DNA	$C_7H_6N_2O_5$	20			
60	FOX-7	$C_2H_4N_4O_4$	70	$C_{2.00517}H_{2.799119}N_{2.193502}O_{2.64771}$	−44.19	7.974
	DNA	$C_7H_6N_2O_5$	30			

Table 2
Abbreviation of explosives and their corresponding name, structure

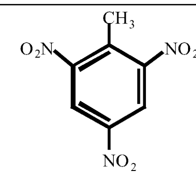
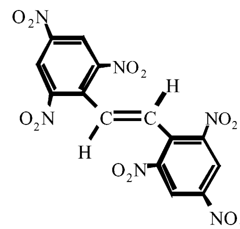
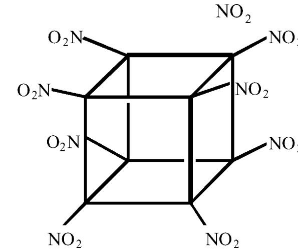
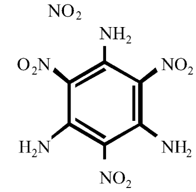
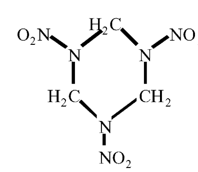
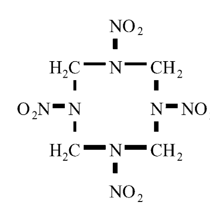
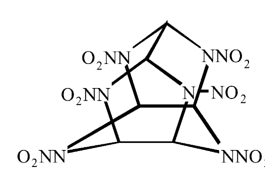
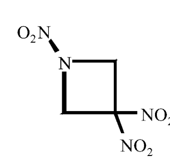
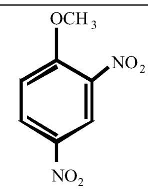
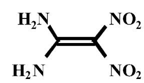
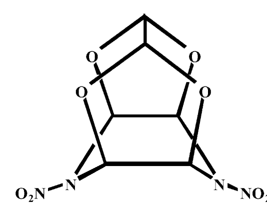
S. no.	Name of the HEM	Abbreviation	Molecular formula	Structure	Velocity of detonation (km/s)		
					Literature	LOTUSES	Deviation
1	2,4,6-Trinitrotoluene	TNT	$C_7H_5N_3O_6$		6.9	6.66456	0.23544
2	*Trans*-2,2′,4,4′,6,6′-hexanitrostilbene	HNS	$C_{14}H_6N_6O_{12}$		7.12	6.82942	0.29058
3	Octanitrocubane	ONC	$C_8N_8O_{16}$		9.9	9.0588	0.8412
4	1,3,5-Triamino-2,4,6-trinitrobenzene	TATB	$C_6H_6N_6O_6$		7.94	7.86086	0.07914
5	Cyclotrimethylenetrinitramine	RDX	$C_3H_6N_6O_6$		8.85	8.93981	−0.08981
6	Cyclotetramethyl-enetetranitramine	HMX	$C_4H_8N_8O_8$		9.1	9.04212	0.05788
7	Ammonium nitrate	AN	$H_4N_2O_3$	NH_4NO_3	5.27	7.3442	−2.0742
8	Hexanitrohexa-azaisowurtzitane	CL-20	$C_6H_6N_{12}O_{12}$		9.4	9.3808	0.0192
9	1,3,3-Trinitroazetidine	TNAZ	$C_3H_4N_4O_6$		8.5	8.6763	−0.1763

Table 2 (*Continued*)

S. no.	Name of the HEM	Abbreviation	Molecular formula	Structure	Velocity of detonation (km/s)		
					Literature	LOTUSES	Deviation
10	2,4-Dinitroanisole	DNA	$C_7H_6N_2O_5$		6.74	5.7057	1.0343
11	1,1-Diamino-2,2-dinitro-ethylene	FOX-7	$C_2H_4N_4O_4$		9.09	8.7351	0.3549
12	Tetraoxa explosive 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo-(5.5.0.05,9 03,11)dodecane	TEX	$C_6H_6N_4O_8$		8.665	7.8210	0.844

3. Results and discussion

Computer code named LOTUSES-1.4 is developed to optimize the mixed explosive composition to get maximum output performance. The approach involved in the development of code comprises two important steps: (i) optimization of the oxygen balance of the ingredients and (ii) prediction of maximum possible detonation velocity for mixed explosive composition. The algorithm written in LOTUSES-1.4 by the author, vary the composition of mixed explosives automatically in the range of 1–100% and computes the oxygen balance as well as the velocity of detonation for various compositions in preset steps. At the end of several iterations performed by LOTUSES-1.4, it automatically gives the optimized composition of mixed explosive for which maximum output performance of mixed explosive is expected.

Most of the military explosives are solid compositions, which are made up of two explosive components. Generally two different techniques are followed to make military explosive compositions, namely: (i) melt casting and (ii) pressing. Explosive compositions which are processed by melt casting are generally contains TNT, which has a relatively low melting temperature (80 °C) compared with its ignition temperature (240 °C). In this paper, we report a variety of melt cast explosive formulations with their predicted performance properties at different compositions. The velocity of detonation and oxygen balance data generated by LOTUSES (Version 1.4) for high explosives like RDX, HMX, ONC, CL-20, TATB, HNS, TEX, FOX-7 with low melting ingredients like TNT, DNA and TNAZ at different compositions are presented in Table 1. The variation of velocity of detonation with increase in the composition of ammonium nitrate (AN) is shown in Fig. 1. The data in Fig. 1 shows that the velocity of detonation of mixed explosive is greater than the individual component at 80:20 composition, which is confirmed by the reported in literature [23]. In Fig. 2, oxygen balance and velocity of detonation of AN:TNT mixture at different composition is plotted along *X* and *Y* axis, respectively. The results depicted in Fig. 2 and Table 1 reveals that, when the oxygen balance of mixed explosive composition approaches towards zero, their velocity of detonation increases. Abbreviation of explosives and their corresponding name, structures are given in Table 2. Also Table 2 presents the comparison of velocity of detonation for pure explosives generated using LOTUSES (Version 1.4) with reported in literatures [23,25,26,37–41].

4. Conclusion

An algorithm to compute the performance properties of mixed explosive composition is developed and successfully incorporated to the existing LOTUSES code. The computer code has been validated with well-known explosive RDX, HMX, ONC, CL-20, TATB, HNS, TEX, FOX-7 with low melting ingredients like TNT, DNA and TNAZ at different compositions. LOTUSES also can predict the velocity of detonation, density, C–J pressure, heat of explosion, heat of formation, volume of explosion of gaseous products, etc., the new algorithm incorporated enhances its efficiency and makes it a more powerful tool for the scientists/researches working in the field of high energy materials. Finally, it is concluded that the new algorithm incorporated in LOTUSES (Version 1.4) will allow theoretical screening of notional hazardous materials for identification of promising mixed explosive compositions for additional study and elimination of weaker candidates from further consideration. Thereby, reducing cost associated with the development programme of the high energy materials.

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