

# Computer simulation for prediction of performance and thermodynamic parameters of high energy materials

H. Muthurajan<sup>a</sup>, R. Sivabalan<sup>b</sup>, M.B. Talawar<sup>b,\*</sup>, S.N. Asthana<sup>b</sup>

<sup>a</sup> Armament Research and Development Establishment, Pashan, Pune 48 021, India

<sup>b</sup> High Energy Materials Research Laboratory, Sutarwadi, Pune 48 021, India

Received 3 December 2003; received in revised form 18 April 2004; accepted 19 April 2004

Available online 7 June 2004

## Abstract

A new code viz., Linear Output Thermodynamic User-friendly Software for Energetic Systems (LOTUSES) developed during this work predicts the theoretical performance parameters such as density, detonation factor, velocity of detonation, detonation pressure and thermodynamic properties such as heat of detonation, heat of explosion, volume of explosion gaseous products. The same code also assists in the prediction of possible explosive decomposition products after explosion and power index. The developed code has been validated by calculating the parameters of standard explosives such as TNT, PETN, RDX, and HMX. Theoretically predicated parameters are accurate to the order of  $\pm 5\%$  deviation. To the best of our knowledge, no such code is reported in literature which can predict a wide range of characteristics of known/unknown explosives with minimum input parameters. The code can be used to obtain thermochemical and performance parameters of high energy materials (HEMs) with reasonable accuracy. The code has been developed in Visual Basic having enhanced windows environment, and thereby advantages over the conventional codes, written in Fortran. The theoretically predicted HEMs performance can be directly printed as well as stored in text (.txt) or HTML (.htm) or Microsoft Word (.doc) or Adobe Acrobat (.pdf) format in the hard disk. The output can also be copied into the Random Access Memory as clipboard text which can be imported/pasted in other software as in the case of other codes. © 2004 Elsevier B.V. All rights reserved.

**Keywords:** Computational modeling; Detonation velocity; Heat of explosion; Chapman–Jouguet (C–J) pressure; Volume of explosion products; Hazardous materials

## 1. Introduction

Intensive search is on all over the globe to develop new high energy materials (HEMs) to meet the futuristic needs. With the advancement of information technology and revolution in the dissemination of scientific information through World Wide Web network, scientists and technologists are making dedicated efforts to explore the knowledge and expertise available in the area of information technology for application in the field of HEMs. This will lead to quantum jump in the advancement of science and technology of HEMs. Of particular importance in designing new explosives, is the ability to predict performance of compounds before the laborious and expensive task of synthesizing them [1]. Rigorous mathematical approaches developed at present, allow one to formalize the knowledge of spe-

cialists in synthesis [2]. The search of energetic materials is best carried out presently using thermodynamics and molecular engineering approaches, which help in designing efficient materials. In recent past, theoretical calculations to predict detonation behavior of explosives have evinced great interest [3–5]. Theoretical screening of notional materials allows for identification of promising candidates for additional study and elimination of poor candidates from further consideration, and thus, reducing costs associated with synthesis, and evaluation of the materials [1]. This capability leads to better designs and shorter design cycles. One of the most important parameters used during performance parameters calculation is the density and the most widely used manual method currently available in literature for its prediction is the Stine's method [1]. The two most widely used versatile codes to calculate detonation properties are CHEETAH and TIGER [6]. The former is available only to limited agencies while the latter is available commercially.

\* Corresponding author. Tel.: +91-20-5869-316.

E-mail address: mbtalawar@yahoo.com (M.B. Talawar).

This paper documents an integrated code named Linear Output Thermodynamic User-friendly Software for Energetic Systems (LOTUSES), which is based on the known logic and has been validated with the experimentally obtained values for well-established explosives. The main objective of this research was to conduct a retrospective analysis of theoretical approaches of estimating the explosive detonation parameters and to make a theoretical performance prediction for a number of promising HEMs based on the currently used calculation methods. The explosives ranging from nitroaromatics, cyclic and linear nitramines, nitrate esters, nitro-nitrato aliphatics and zero hydrogen explosives were studied and results obtained are presented in this paper. Various numerical methods that were developed in the last two decades following World War II onwards have been analyzed to develop this software. It combines Stine's approaches to compute density, KW rule [7] for predicting possible decomposition products and Rothstein's method [8] for predicting detonation factor as well as velocity of detonation (VOD) and Cooper method [9] for estimating C–J pressure. In this article, we describe the use of computational approach in predictions of the heats of detonation, heat of explosion, volume of explosion products gases of various HEMs.

## 2. Prediction of HEMs parameters

### 2.1. Balancing explosion reaction process

A great quantity of energy deposited into a relatively small volume, manifests itself by a rapid expansion of hot gases, which in turn can create a shock wave or propel fragments outwards at high speed. Chemical explosions may be distinguished from other exothermic reactions by the extreme rapidity of the reactions. In addition to the violent release of energy, chemical explosions must provide a means to transfer the energy into mechanical work. This is accomplished by readily expanding the product gases.

In order to perform detonation parameter calculations, one must know the detonation products. Most chemical explosions involve a limited set of simple reactions, all of which involve oxidation (reaction with oxygen). A relatively easy way to balance chemical explosive equations is to assume that the following partial reactions take place to the max-

imum extent (meaning one of the reactants is totally consumed) and in order of precedence. To predict the problem of decomposition products, a set of rules was developed by Kistiakowsky and Wilson [7]. These rules are being used currently for moderately oxygen-deficient explosives ( $-40\% > OB$ ). The Kistiakowsky–Wilson [7] rules are presented in Table 1.

### 2.2. Estimation of density

One property of the compound that is helpful in evaluating an explosive's performance is its density. Various experiments show that the detonation velocity of one-component explosives increases with increasing density [9,10]. Thus, density is one of the parameter of prime importance and its prediction should be as accurate as possible. Recently, the prediction of density was made by empirical equations based on the volume additivity procedures [1].

Several methods are reported to estimate the density [1,6] of a compound and can be divided roughly into two broad categories: those of theoretical nature and those of an empirical nature. The theoretical approach uses detailed information about the crystal structure in calculating density of a compound. That is, the density of an organic compound can be calculated on a fundamental basis if all inter- and intra-molecular forces are known. This method has the dual advantages that structures for different polymorphs can be calculated as well as unique bonding patterns such as hydrogen bonding or conjugation can be considered. Although, the inter- and intra-molecular forces for these large organic compounds are not well characterized and their calculations are extremely complex, such methods of predicting density are being pursued by the authors and will be reported elsewhere in future.

Alternatively, the density of a compound can be estimated by adopting an empirical approach. The molar volume of a compound usually is assumed to be a linear combination of the volumes of its constituent chemical entities, such as  $-NO_2$ ,  $-OH$ ,  $-NH_2$  or of its atoms. Of course, the molar volume is only approximately additive and is complicated by steric effects, conjugation, and ring systems, etc. However, enormous experimental crystallographic data suggest that atoms in similar bonding situations have similar bond lengths, bond angle and dihedral angles, and hence, would occupy similar volumes. The empirical method used in the

Table 1  
Kistiakowsky–Wilson hierarchy rules—priorities of explosive reactions

Priority	Condition	Reaction (to completion)
1	Carbon atoms are converted to carbon monoxide	$C + O \rightarrow CO$ (gas)
2	If any oxygen remains then hydrogen is oxidized to water	$2H + O \rightarrow H_2O$ (gas)
3	If any oxygen still remains then carbon monoxide is oxidized to carbon dioxide	$CO + O \rightarrow CO_2$ (gas) (the CO comes from reaction (1)) $2O \rightarrow O_2$ (gas)
4	Excess of O, H and N is converted to $O_2$ , $H_2$ and $N_2$	$2H \rightarrow H_2$ (gas) $2N \rightarrow N_2$ (gas)

present work, describes a simple approach of predicting the molar volume of a crystalline compound, along with sufficient error analysis to set confidence limits on the predicted density.

The molar volume,  $V$  is assumed to be a linear combination of the constituent volumes,  $v_i$ . That is for the  $j$ th compound

$$v_j = \sum_{i=1}^n a_{ij} v_n \quad (1)$$

or in matrix notation

$$V = Av + \varepsilon \quad (2)$$

where  $A$  is the coefficient matrix (and  $a_{ij}$  are its elements). The vector of the deviations between the observed and calculated molar volumes,  $\varepsilon$  is needed to make the equations consistent. In this method, crystallographic unit cell dimensions are given in unit of angstroms ( $\text{\AA}$ ), and thus, crystal volumes ( $\text{\AA}^3$  per molecule) rather than molar volumes ( $\text{cm}^3/\text{mol}$ ) were fitted. The conversion between them is  $V_{\text{crystal}}$  ( $\text{\AA}^3$  per molecule) =  $0.6023V_{\text{molar}}$  ( $\text{cm}^3/\text{mol}$ ).

For example, a carbon atom that forms two single bonds and one double bond is differentiated from a carbon atom that forms two aromatic bonds and a single bond. To aid to the specifications of the atom's bonding environment, we denote a single, double, and triple bond by 1, 2, and 3, respectively, and if the bonds are part of the ring system, by  $-1$ ,  $-2$ , and  $-3$ , respectively. An aromatic bond (as in benzene) is denoted by  $-5$  as it also must be a part of ring system. Conjugated bonds are denoted by 7 or  $-7$ , the latter if the bond is part of the ring system. Thus, O (2) represents an oxygen atom with one double bond, O (1, 1) two single bonds, and O ( $-1$ ,  $-1$ ) two single bonds that are also part of a ring system. Some of the bonding environments correspond to extremely rare situations, such as C ( $-1$ ,  $-1$ ), C ( $-2$ ,  $-2$ ) or N (1, 1, 1, 1) and some of these are grouped together.

### 2.3. Velocity of detonation (VOD) analysis

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. The detonation velocity is the rate of propagation of a shock wave in an explosive. The VOD is directly dependent on the density of a given explosive and is not influenced by external factors [11]. This is true for ideal explosives (explosives that attain nearly maximum performance in very small diameters). A simple, empirical linear relationship between detonation velocity at theoretical maximum density and detonation factor ( $F$ ) that is dependent solely upon chemical composition and structure is postulated for ideal C, H, N, O type explosives by Rothstein

and Petersen [8,12]. The detonation factor  $F$  is expressed as

$$F = 100 \times \frac{nO + nN - (nH/2nO) + (A/3) - (nB/1.75) - (nC/2.5) - (nD/4) - (nE/5)}{MW} - G \quad (3)$$

$$D = \frac{F - 0.26}{0.55} \quad (4)$$

where  $nH$ ,  $nN$ ,  $nO$  are number of hydrogen, nitrogen, and oxygen atoms in a molecule (users need not to enter separately in LOTUSES, it will be taken from the empirical formula entered by the user),  $nB$  is number of oxygen atoms in excess of those already available to form  $\text{CO}_2$  and  $\text{H}_2\text{O}$  (in the LOTUSES user need not to give  $nB$  input parameter, since it is being calculated directly from the molecular formula in situ during explosive decomposition product analysis),  $nC$  number of oxygen atoms doubly bonded directly to carbon as in carbonyl,  $nD$  number of oxygen atoms singly bonded directly to carbon,  $nE$  number of nitro groups existing either as in a nitrate ester configuration or as a nitric acid salt such as hydrazine mono nitrate,  $A = 1$  if the compound is aromatic otherwise  $A = 0$ ,  $G = 0.4$  for liquid explosive, and  $G = 0$  for solid explosive,  $F$  the detonation factor, and  $D$  is the detonation velocity.

### 2.4. Predicting Chapman–Jouguet (C–J) pressure

It is necessary in many explosives engineering calculations to know the value of the C–J state pressure and  $P_{\text{Cj}}$  of a particular explosive of interest. Of course, one may conduct a series of experiments to determine  $P_{\text{Cj}}$  at the desired density. However, such experiments are difficult to conduct and are expensive and time consuming.

Kamlet and Abland [13] showed simple relations for the detonation velocity and C–J pressure which can be used to fit numerical data resulting from a complex computer code. These simple relations, which are valid for C–H–N–O explosives, depend on moles of detonation gas per unit weight of explosive, average molecular weight of these gases, chemical energy of the detonation reaction and density [14–18]. The correlation of a broad experimental data base yields a power function relationship between Chapman–Jouguet (C–J) pressure and density. This function in combined with the Rankine-Hugoniot equations for mass and momentum. An equation can be derived to estimate C–J pressure simply. The estimating equation [13] is as follows:

$$P_{\text{Cj}} = \rho_0 D^2 (1 - 0.713 \rho_0^{0.07}) \quad (5)$$

where  $P_{\text{Cj}}$  is the pressure of the detonation product gases at the C–J state (GPa),  $\rho_0$  the initial density of the unreacted explosive ( $\text{g}/\text{cm}^3$ ), and  $D$  is the detonation velocity (km/s).

### 2.5. Predicting heat of explosion

The heat of explosion is a quantity used to assess a hazardous materials' detonation performance [19]. The heat of explosion,  $Q$ , defined as the negative of the enthalpy change of the detonation reaction, is the energy available to do mechanical work and has been used to estimate potential damage to surroundings. Before embarking upon the synthesis or formulation of new energetic materials, the chemist needs to estimate the performance properties in order to evaluate the potential of the approach [6]. The process has two steps: (1) one must estimate the heat of formation if the formulation contains one or more compounds for which this property is unknown. (2) Using the heat of formation of individual ingredients as one of the input parameters, the performance properties (e.g. temperature of combustion, product distribution, velocity of detonation, etc.) are calculated using a computer code. The total amount of energy released in a explosion reaction by one mole of reactant is called the heat of explosion. It can be calculated by comparing the heats of formation before and after the reaction.

The net heat difference between heats of formations of the reactants and products in a chemical reaction is termed the heat of reaction. For oxidation, this heat of reaction may be termed heat of combustion. In explosive technology only materials that are exothermic that is, have a heat of reaction that causes net liberation of heat are of our interest. Hence, in this text, heats of reactions are virtually all positive. Since reactions may occur either under conditions of constant pressure or constant volume, the heat of reaction can be expressed at constant pressure or at constant volume. It is this heat of reaction that may be properly expressed as "heat of the explosion". Explosion being exothermic phenomenon the value is always positive. The amount of energy released by 1 kg of explosive can be computed from heat of detonation and molecular weight of reactant. From the empirical formula given by the user our software could accurately calculate the molecular weight of the reactant and renders it is possible to predict the heat of detonation.

$$\begin{aligned} \text{Amount of energy released (kJ/kg)} \\ = \frac{1000 \times \text{Heat of detonation (kJ/mol)}}{\text{Molecular weight}} \end{aligned} \quad (6)$$

### 2.6. Predicting volume of products of explosion

The law of Avogadro states that equal volumes of all gases under the same conditions of temperature and pressure contain the same number of molecules. From this law, it follows that the molecular volume of one gas is equal to the molecular volume of any other gas. The molecular volume of any gas at 0 °C and under normal atmospheric pressure is very nearly 22.41 or 22.4 dm<sup>3</sup>. Newly developed software will automatically balance the explosion reaction of HEMs

based on Kitioswasky–Wilson rules and predicts the explosion products. From the number of moles of explosion products, it could possible to calculate the volume of explosion products.

### 2.7. Estimation of power index

In an explosive reaction, heat and gases are liberated. The volume of gas  $V$  and the heat of explosion  $Q$  can both be calculated independently but these values can be combined to give the value for the explosive power [5] as shown in the following equation:

$$\text{Explosive power} = QV \quad (7)$$

The value for the explosive power is then compared with the explosive power of a standard explosive (picric acid) to obtain power index, as shown in the following equation, where data for  $Q_{(\text{picric acid})}$  and  $V_{(\text{picric acid})}$  are 3250 kJ/g and 0.831 dm<sup>3</sup>, respectively

$$\text{Power index} = \frac{QV}{Q_{(\text{picric acid})}V_{(\text{picric acid})}} \times 100 \quad (8)$$

### 2.8. About software design

Graphical User Interfaces (GUIs), have revolutionized the microcomputer industry. They demonstrate that the proverb, "A picture is worth a thousand words", has not lost its truth to most computer users. Therefore, it is essential to develop programs for any version of Windows. Hence, we have chosen Visual Basic 6.0 as an efficient application tool to develop this numerical modeling software. In particular, Visual Basic could add menus, text boxes, command buttons, option buttons (for making exclusive choices), check boxes (for non-exclusive choices), list boxes, scroll bars, as well as file and directory boxes to blank windows. One can use grids to handle tabular data and can communicate with other Windows applications. Visual Basic has multiple toolbars, which could be customized to easily build one's own toolbar to suit the needs as well as multiple windows on a screen. The currently developed software code can be used simultaneously in execution with other softwares. As soon as the Login procedure is completed, the screen which appears to the user is termed as Simulation Screen. The tool bar and brief action of each tools of LOTUSES is illustrated (Fig. 1).

The LOTUSES based on computational technique is designed by us in such a way that it can run in windows 95/98/XP operating systems. It is highly compatible for Local Area Network (LAN) also. The empirical formula and the heat of formation are the inputs to the LOTUSES 1.2, with this information it can predict the heat of detonation, heat of explosion, volume of the gaseous products and other vital parameters of both aromatic and non-aromatic organic HEMs.

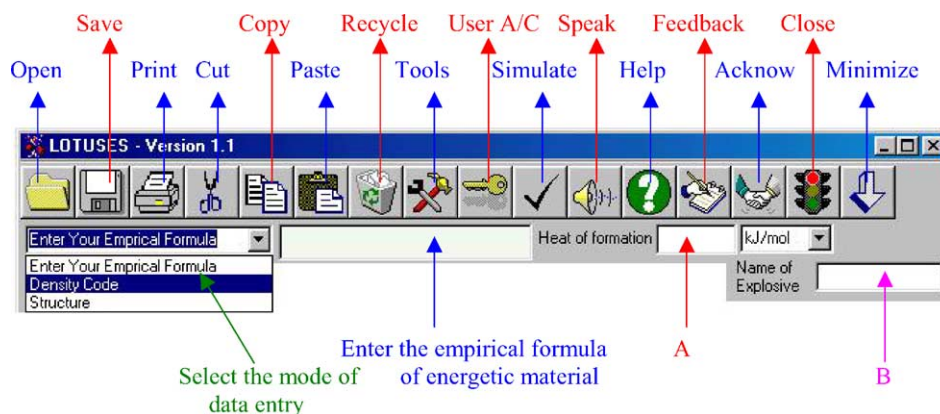


Fig. 1. Tool bar of newly developed LOTUSES code.

Brief description of individual tool represented in the tool bar of LOTUSES are as follows:

OPEN	Open a text file and display the content.
SAVE	Save the simulated output in secondary memory devices (hard disk, floppy drives, compact disk, etc.) in required format (.txt, .doc, .htm).
PRINT	Sends the simulated output to the printing devices. If Acrobat .pdf writer software is installed on PC, then the printing output can be stored in .pdf format also.
CUT	Cut the explosive simulated information from the LOTUSES, which can be pasted/imported in any other windows applications.
COPY	Copy the explosive simulated information from the LOTUSES, which can be pasted/imported in any other windows applications.
PASTE	Paste the text information available in clipboard to LOTUSES for simulation.
RECYCLE	Clears the content of LOTUSES.
TOOLS	Default setting of the software can be modified by the user, such as background color, font type, font size, data base, etc.
USER A/C	Add/delete/modify users account for the proper utilization of this software and track their activity.
SIMULATE	Simulate the explosive modeling computer codes.
SPEAK	Send the output of explosive modeling in audio format to the multimedia speakers.
HELP	Help menu will appear on the screen.
ACKNOW	Acknowledgement screen will be displayed.
CLOSE	Close the application.
MINIMIZE	Minimize the application and can be activated at any time.

### 3. Results and discussion

#### 3.1. Performance parameters of HEMs

Molecular weights and atomic compositions for explosives were derived, respectively, from the sum of the weighed average molecular weights and the weighed average sums of each elemental mole fraction, which were automatically calculated by the software from the molecular formula. The explosives ranging from nitro aromatics, cyclic, and linear nitramines, nitrate esters and nitro-nitrato aliphatics and zero hydrogen explosives were studied in the present work. Predicted density and corresponding experimentally observed density of 72 HEMs are tabulated in Table 2. A linear straight line having  $R^2$  as 0.83 with straight-line equation of  $y = 0.77x + 0.42$  was obtained on plotting (Fig. 2) experimentally determined density reported in literature along the  $x$ -axis and predicted density by LOTUSES along the  $y$ -axis.

Fig. 3 reflects the error analysis on deviation between the experimentally observed density and that

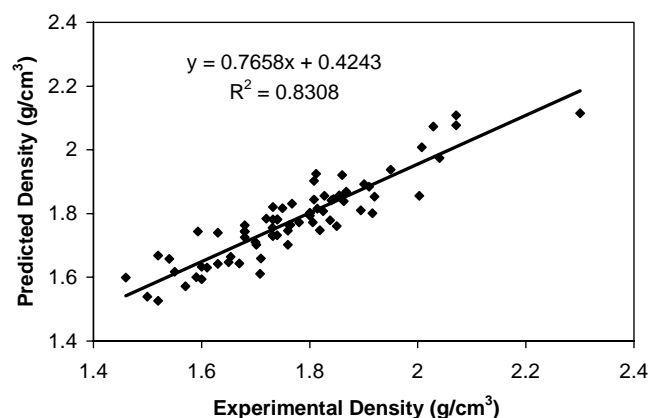


Fig. 2. Experimental vs. predicted density ( $\text{g}/\text{cm}^3$ ).

Table 2  
Comparison of predicted and observed density

Serial number	Name of explosive	Empirical formula	Molecular weight (LOTUSES)	Density (g/cm <sup>3</sup> ) (LOTUSES)	Observed density (g/cm <sup>3</sup> )	Error (%)
1	Diglycerol tetranitrate	C <sub>6</sub> H <sub>10</sub> N <sub>4</sub> O <sub>13</sub>	346.2	1.66	1.52	-9.75
2	Metriol trinitrate	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> O <sub>9</sub>	255.2	1.59	1.46	-9.52
3	NG	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub>	227.1	1.74	1.593	-9.48
4	Penta erythritol tri nitrate (PETRIN)	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> O <sub>10</sub>	271.2	1.65	1.54	-7.67
5	Diazodinitrophenol	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>5</sub>	210.1	1.74	1.63	-6.76
6	ADN	H <sub>4</sub> N <sub>4</sub> O <sub>4</sub>	124.1	1.92	1.812	-6.19
7	1,4-Diamino-2,5-dinitro imidazole	C <sub>3</sub> H <sub>4</sub> N <sub>6</sub> O <sub>4</sub>	188.1	1.90	1.808	-5.25
8	DADN	C <sub>4</sub> H <sub>4</sub> N <sub>4</sub> O <sub>5</sub>	188.9	1.82	1.732	-5.8
9	Nnitro isobutyltrinitrate (NIBTN)	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	286.1	1.76	1.68	-4.93
10	Ethyl picrate	C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>7</sub>	257.2	1.61	1.55	-4.33
8	Trinitro benzoic acid	C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> O <sub>8</sub>	257.1	1.81	1.75	-3.79
12	2,4,6-Trinitro- <i>m</i> -cresol	C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>7</sub>	243.1	1.74	1.68	-3.77
13	Trinitro cresol (TNC)	C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	227.1	1.74	1.68	-3.77
14	Ammonium picrate (XPL-D)	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>7</sub>	246.2	1.78	1.72	-3.74
15	Picric acid	C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>	229.9	1.83	1.767	-3.63
16	HNF	CH <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	183.1	1.92	1.86	-3.24
17	Diaminodinitro pyrrole	C <sub>4</sub> H <sub>5</sub> N <sub>5</sub> O <sub>4</sub>	187.1	1.78	1.732	-2.87
18	Trinitrophenoxy ethylnitrate (TNPON)	C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>10</sub>	318.2	1.72	1.68	-2.72
19	Trimethyloethylmethane trinitrate or ethriol trinitrate	C <sub>6</sub> H <sub>8</sub> N <sub>3</sub> O <sub>9</sub>	269.2	1.54	1.5	-2.64
20	1,3,5-Trinitro-2,4,6-triamio triazine	C <sub>3</sub> H <sub>9</sub> N <sub>9</sub> O <sub>6</sub>	267.2	1.78	1.74	-2.40
21	1,3,5,7-Tetranitro-2,4,6,8-tetraamino 1,3,5,7-tetrazaoctane	C <sub>4</sub> H <sub>12</sub> N <sub>12</sub> O <sub>8</sub>	356.3	1.78	1.7405	-2.37
22	1,4-Dinitro-difurazanopiperazine	C <sub>4</sub> N <sub>8</sub> O <sub>6</sub>	256.1	2.07	2.029	-2.19
23	Dinitrophenoxyethylnitrate (DNPEN)	C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>8</sub>	273.2	1.63	1.6	-2.06
24	1,3,5-Trinitro-2,4,6-hexafluoroamino-1,3,5-triazahexane	C <sub>3</sub> H <sub>3</sub> N <sub>9</sub> O <sub>6</sub> F <sub>6</sub>	375.1	2.12	2.078	-1.82
25	3-Amino-5-nitro-1,3,4-oxadiazole	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	130.1	1.86	1.827	-1.55
26	TETRYL	C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>8</sub>	287.2	1.76	1.731	-1.40
27	Diaminofurazan	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> O	100.1	1.63	1.61	-1.30
28	Dipenta erythritol hexa nitrate (DIPEHN)	C <sub>10</sub> H <sub>16</sub> N <sub>6</sub> O <sub>19</sub>	524.3	1.64	1.63	-0.74
29	Tetramethylol cyclopentanone (FIVONITE)	C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O <sub>13</sub>	384.2	1.61	1.59	-0.70
30	TNT	C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	227.1	1.66	1.654	-0.66
31	PETN	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub>	316.2	1.71	1.7	-0.57
32	2,4-Dinitro toluene (DNT)	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	182.1	1.52	1.52	-0.41
33	1,3,5,7-Tetranitro-2,4,6,8-octafluoroamino-3,5,7-tetrazaoctane	C <sub>4</sub> H <sub>4</sub> N <sub>12</sub> O <sub>8</sub> F <sub>8</sub>	500.2	2.08	2.078	-0.27
34	Mannitol hexa nitrate	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>18</sub>	452.2	1.80	1.8	-0.14
35	1,4-Dinitro-piperazine	C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	176.1	1.57	1.57	-0.13
36	Hexanitro diphenyl oxide (HNDPO)	C <sub>12</sub> H <sub>4</sub> N <sub>6</sub> O <sub>13</sub>	440.2	1.81	1.814	-0.09
37	Diaminotrinitropyridine	C <sub>5</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>	244.1	1.85	1.844	-0.09
38	Hexanitrodiphenylamine (HNDP)	C <sub>12</sub> H <sub>5</sub> N <sub>7</sub> O <sub>12</sub>	439.2	1.80	1.8	-0.08
39	Tetraoxa explosive (TEX)	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	262.2	1.86	1.855	-0.08
40	Hexanitro-tetraaminebiphenyl ether	C <sub>12</sub> H <sub>8</sub> N <sub>10</sub> O <sub>13</sub>	500.3	1.84	1.84	-0.08
41	Diaminotrinitrotoluene	C <sub>7</sub> H <sub>7</sub> N <sub>5</sub> O <sub>6</sub>	257.2	1.70	1.7014	-0.07
42	Trinitroaniline (TNA)	C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>6</sub>	228.1	1.76	1.762	-0.07
43	Hexanitro tetramine stilbene	C <sub>14</sub> H <sub>10</sub> N <sub>10</sub> O <sub>12</sub>	510.3	1.77	1.764	-0.07
44	Hexanitrobenzene (HNB)	C <sub>6</sub> N <sub>6</sub> O <sub>12</sub>	348.1	2.00	2.007	-0.06
45	Keto-RDX	C <sub>3</sub> H <sub>4</sub> N <sub>6</sub> O <sub>7</sub>	236.1	1.87	1.8678	-0.06
46	2,3,4,6-Tetra nitro aniline	C <sub>6</sub> H <sub>3</sub> N <sub>5</sub> O <sub>8</sub>	273.1	1.86	1.867	0.12
47	Ethylendinitramine (EDNA)	C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub>	150.1	1.64	1.65	0.18
48	DNDNPy	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O <sub>4</sub>	199.1	1.73	1.732	0.18
49	Poly vinyl nitrate (PVN)	C <sub>2</sub> H <sub>3</sub> NO <sub>3</sub>	89.1	1.59	1.6	0.39
50	Triaminotrinitrobenzene (TATB)	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	258.2	1.79	1.8	0.40
51	HMX	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	296.2	1.77	1.78	0.40
52	HNS	C <sub>14</sub> H <sub>6</sub> N <sub>6</sub> O <sub>12</sub>	450.3	1.73	1.74	0.43
53	Dinitroglyco urile (DINGU)	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>	232.1	1.89	1.908	0.44
54	Tetranitroglyco urile (SORGUYL)	C <sub>4</sub> H <sub>2</sub> N <sub>8</sub> O <sub>10</sub>	322.1	1.94	1.95	0.65
55	Trinitro benzene (TNB)	C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub>	213.9	1.75	1.76	0.81
56	4,5-Bispiacrylamino-4,6-dinitro benzene	C <sub>17</sub> H <sub>7</sub> N <sub>8</sub> O <sub>16</sub>	621.4	1.81	1.825	0.99
57	Diaminotrinitro benzoic acid	C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>8</sub>	287.2	1.84	1.863	1.31
58	Dinitroazofuroxan (DNAF)	C <sub>4</sub> N <sub>8</sub> O <sub>8</sub>	288.1	1.88	1.91	1.34
59	Dioxy ethyl nitramine dinitrate (DINA)	C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>8</sub>	240.1	1.64	1.67	1.60
60	RDX	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	222.1	1.77	1.806	1.83
61	Nitroguanidine	CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	104.1	1.66	1.71	3.01

Table 2 (Continued)

Serial number	Name of explosive	Empirical formula	Molecular weight (LOTUSES)	Density (g/cm <sup>3</sup> ) (LOTUSES)	Observed density (g/cm <sup>3</sup> )	Error (%)
62	CL-20	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	438.2	1.97	2.04	3.20
63	Diaminotrinitrobenzene (DATB)	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	243.2	1.78	1.838	3.22
64	DAAT	C <sub>4</sub> H <sub>4</sub> N <sub>12</sub>	220.2	1.70	1.76	3.28
65	NTO	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	130.1	1.85	1.92	3.45
66	TADNPy	C <sub>5</sub> H <sub>6</sub> N <sub>6</sub> O <sub>4</sub>	214.2	1.75	1.819	3.89
67	3,5-Diamin ammonium picrate	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>7</sub>	276.2	1.81	1.895	4.47
68	Tetranitrodibenzo tetrazapentalene (TACOT)	C <sub>12</sub> H <sub>4</sub> N <sub>8</sub> O <sub>8</sub>	388.2	1.76	1.85	4.82
69	Methyl nitrate	CH <sub>3</sub> NO <sub>3</sub>	77.0	1.68	1.708	5.66
70	Tetranitropyrazine	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	296.2	1.80	1.916	6.03
71	Aminonitro furazan	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	130.1	1.86	2.003	7.37
72	Octa nitro cubane (ONC)	C <sub>8</sub> N <sub>8</sub> O <sub>16</sub>	464.12	2.85	2.3	8.05

predicted by LOTUSES. From the bar diagram, it is clear that out of 72 HEMs taken for theoretical prediction of density analysis, ~96% of the predicted HEMs are within 8% of deviation from the experimental results.

The experimental and predicted results of detonation factor, velocity of detonation and C–J pressure as well as the relative errors of VOD are presented in Table 3. For all data points of velocity of detonation, linear regression analysis yields the identical slope intercept and correlation coefficient,  $R^2$  of 0.9086 with the linear equation  $y = 0.9348x + 0.5027$  (Fig. 4). Thus, the approach developed during this work offers a simple and quick method for estimating detonation pressures at maximum theoretical densities. Fig. 5 reflects the error analysis on deviation between the experimentally determined [8] VOD and that predicted by LOTUSES. From the bar diagram, it is clear that out of 63 HEMs taken for theoretical prediction of velocity of detonation, ~95% of the predicted HEMs are within 6% of deviation from the experimental results (Fig. 5). It is observed that for the same HEM, if it exist in

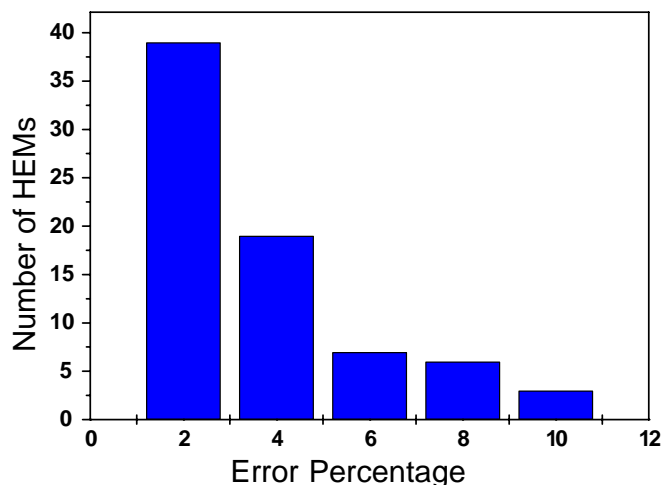


Fig. 3. Error percentage in prediction of density vs. number of HEMs.

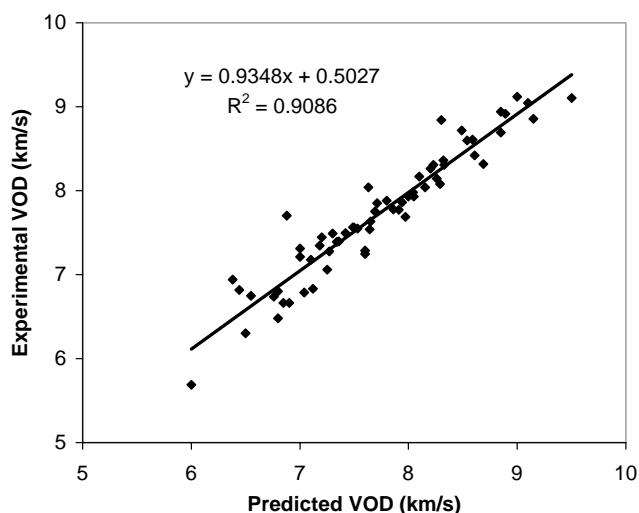


Fig. 4. Experimental vs. predicted velocity of detonation (VOD).

liquid state the value of VOD decreases from that predicted for solid state. Similarly, the value of VOD is lower for the non-aromatic HEM compared to corresponding aromatic analogue.

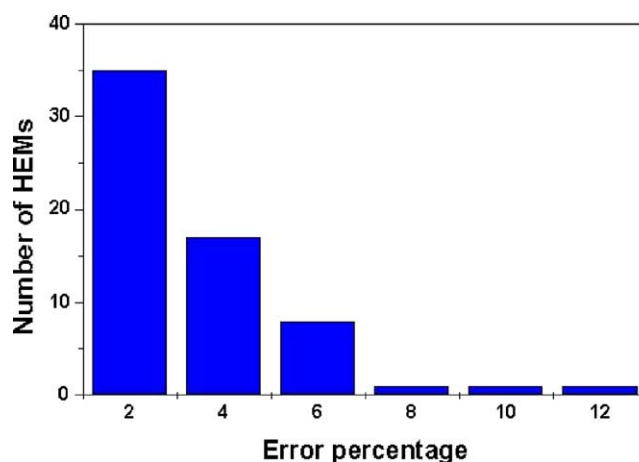


Fig. 5. Error percentage in prediction of VOD vs. number of HEMs.

Table 3  
Comparison of experimental and predicted velocity of detonation

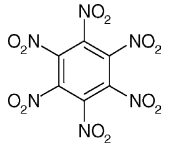
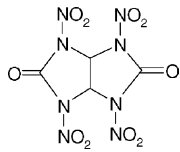
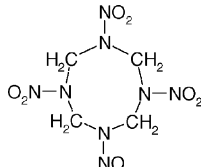
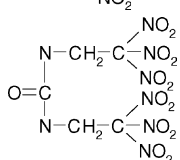
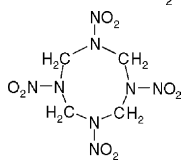
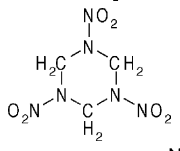
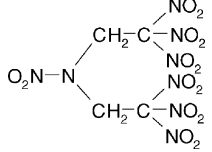
Serial number	Compound	Structure	Empirical formula	Detonation factor		Velocity of detonation (km/s)		Error (%)	C–J pressure (GPa)
				Reported	LOTUSES	Experimental	LOTUSES		
1	HNB		$C_6N_6O_{12}$	5.27	5.266	9.5	9.12	4.2	41.8
2	SORGUYL		$C_4H_2N_8O_{10}$	5.13	5.13	9.15	8.86	3.2	38.7
3	HMX		$C_4H_8N_8O_8$	5.24	5.23	9.1	9.04	0.6	39.5
4	BTNEU		$C_5H_6N_8O_{13}$	5.28	5.28	9	9.87	-1.3	40.7
5	9404		$C_{4.2}H_{8.26}N_{7.73}O_{8.09}$	5.17	5.16	8.89	8.91	-0.3	37.5
6	RDX		$C_3H_6N_6O_6$	5.18	5.17	8.85	8.93	-1.0	37.3
7	BTNEN		$C_4H_4N_8O_{14}$	5.04	5.04	8.85	8.69	1.8	36.6



Table 3 (Continued)

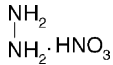
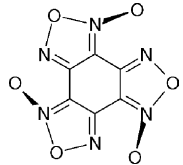
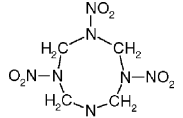
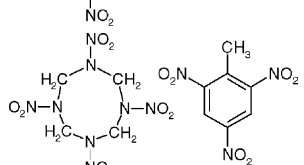
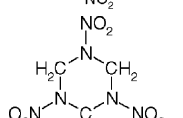
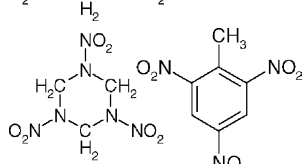
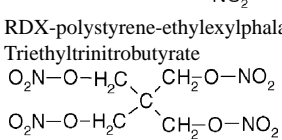
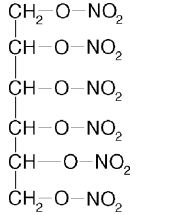
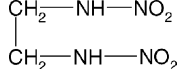
Serial number	Compound	Structure	Empirical formula	Detonation factor		Velocity of detonation (km/s)		Error (%)	C-J pressure (GPa)
				Reported	LOTUSES	Experimental	LOTUSES		
8	HN		H <sub>5</sub> N <sub>3</sub> O <sub>3</sub>	4.88	4.83	8.69	8.31	4.3	29.8
9	BFT		C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	4.89	4.89	8.61	8.42	2.2	30.5
10	908		C <sub>5.12</sub> H <sub>9.41</sub> N <sub>7.55</sub> O <sub>7.73</sub>	4.96	4.99	8.59	8.60	-0.2	33.8
8	OCTOL		C <sub>4.94</sub> H <sub>7.14</sub> N <sub>6.53</sub> O <sub>7.44</sub>	4.88	4.99	8.54	8.59	-0.7	34.4
12	9010		C <sub>3.35</sub> H <sub>5.86</sub> N <sub>5.86</sub> O <sub>5.86</sub>	5.05	5.05	8.49	8.71	-2.7	34.8
13	CYCLOTOL		C <sub>3.96</sub> H <sub>5.73</sub> N <sub>5.24</sub> O <sub>5.98</sub>	4.85	4.83	8.33	8.31	0.3	31.3
14	9205	RDX-polystyrene-ethylhexylphalate	C <sub>4.04</sub> H <sub>6.94</sub> N <sub>5.5</sub> O <sub>5.55</sub>	4.72	4.86	8.32	8.36	-0.5	30.7
15	TNETB	Triethyltrinitrobutyrate	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>14</sub>	4.97	5.12	8.3	8.84	-6.5	30.7
16	PETN		C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub>	4.71	4.70	8.29	8.08	2.6	29.6
17	MHN		C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>18</sub>	4.70	4.74	8.26	8.14	1.4	29.7
18	EDNA		C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub>	4.83	4.83	8.23	8.31	-1.0	29.8

Table 3 (Continued)

Serial number	Compound	Structure	Empirical formula	Detonation factor		Velocity of detonation (km/s)		Error (%)	C–J pressure (GPa)
				Reported	LOTUSES	Experimental	LOTUSES		
19	NQ		CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	4.81	4.80	8.2	8.26	-0.8	30.3
20	DINGU		C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>	4.69	4.68	8.15	8.039	1.4	31.7
21	DNPN	Bis-dinitropropylnitramine	C <sub>6</sub> H <sub>10</sub> N <sub>6</sub> O <sub>10</sub>	4.75	4.75	8.1	8.17	-0.8	30.7
22	COMP B-3		C <sub>4.53</sub> H <sub>5.56</sub> N <sub>4.78</sub> O <sub>5.96</sub>	4.71	4.62	8.05	7.93	1.5	28.4
23	COMP C-4	RDX-polyisobutylene	C <sub>4.02</sub> H <sub>7.82</sub> N <sub>5.44</sub> O <sub>5.55</sub>	4.65	4.65	8.04	7.98	0.7	26.8
24	DINA		C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>8</sub>	4.63	4.62	8	7.94	0.9	24.7
25	TATB		C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	4.59	4.58	7.94	7.86	1.0	30.2
26	TETRYL		C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>8</sub>	4.54	4.53	7.91	7.77	1.8	27.1
27	NIBTN		C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	4.54	4.54	7.86	7.78	1.1	26.5
28	R-SALT		C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>3</sub>	4.60	4.60	7.8	7.89	-1.0	24.9
29	TPEON	Triptaerythritol octanitrate	C <sub>15</sub> H <sub>24</sub> N <sub>8</sub> O <sub>26</sub>	4.29	4.58	7.71	7.85	-1.9	25.0

Table 3 (Continued)

Serial number	Compound	Structure	Empirical formula	Detonation factor		Velocity of detonation (km/s)		Error (%)	C-J pressure (GPa)
				Reported	LOTUSES	Experimental	LOTUSES		
30	NG		$C_3H_5N_3O_9$	4.35	4.25	7.6	7.25	4.6	22.0
31	EDD		$C_2H_{10}N_4O_6$	4.71	4.52	7.69	7.75	-0.8	25.0
32	DATB		$C_6H_5N_5O_6$	4.49	4.49	7.97	7.69	3.5	27.8
33	HNAB		$C_{12}H_4N_8O_{12}$	4.40	4.46	7.65	7.63	0.2	25.9
34	PETRIN		$C_5H_9N_3O_{10}$	4.32	4.41	7.64	7.54	1.3	23.2
35	DNPTB	Dinitropropyl trinitrobutyrate	$C_7H_9N_5O_{12}$	4.50	4.69	7.63	8.04	-5.3	23.8
36	TNPN		$C_8H_6N_4O_{10}$	4.27	4.27	7.6	7.29	4.1	23.3
37	DPEHN		$C_{10}H_{16}N_6O_{19}$	4.41	4.48	7.53	7.55	-0.2	24.3
38	PIC ACID		$C_6H_3N_3O_7$	4.31	4.42	7.5	7.56	-0.8	26.0
39	DIPAM		$C_{12}H_6N_8O_{12}$	4.35	4.43	7.49	7.57	-1.0	26.5
40	TNA		$C_6H_4N_4O_6$	4.38	4.38	7.42	7.496	-1.0	25.6

Table 3 (Continued)

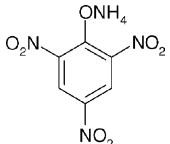
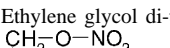
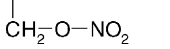
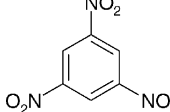
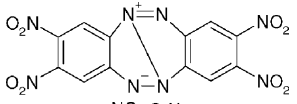
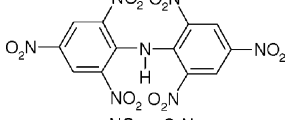
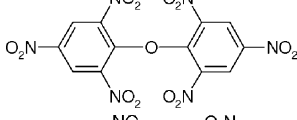
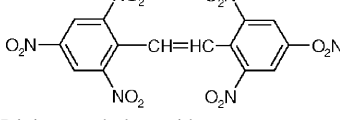
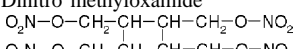
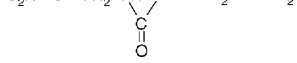
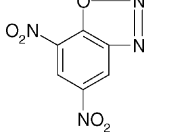
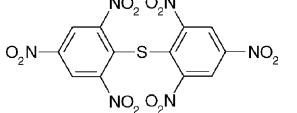
Serial number	Compound	Structure	Empirical formula	Detonation factor		Velocity of detonation (km/s)		Error (%)	C-J pressure (GPa)
				Reported	LOTUSES	Experimental	LOTUSES		
41	XPL D		$C_6H_6N_4O_7$	4.33	4.33	7.36	7.397	-0.5	24.4
42	GTNB	Ethylene glycol di-trinitrobutyrate 	$C_{10}H_{12}N_6O_{16}$	4.31	4.32	7.34	7.39	-0.7	23.8
43	EGDN		$C_2H_4N_2O_6$	4.38	4.38	7.3	7.49	-2.6	22.2
44	TNB		$C_6H_3N_3O_6$	4.26	4.26	7.27	7.28	-0.1	24.1
45	TACOT		$C_{12}H_4N_8O_8$	4.14	4.14	7.25	7.06	2.6	23.6
46	HNDP		$C_{12}H_5N_7O_{12}$	4.36	4.36	7.2	7.44	-3.4	23.4
47	HNDPO		$C_{12}H_4N_6O_{13}$	4.30	4.30	7.18	7.35	-2.3	23.8
48	HNS		$C_{14}H_6N_6O_{12}$	4.02	4.02	7.12	6.83	4.1	21.0
49	DNDMOA	Dinitro methyloxamide 	$C_4H_6N_4O_6$	4.22	4.21	7.1	7.18	-1.1	22.4
50	FIVONITE		$C_9H_{12}N_4O_{13}$	3.99	3.99	7.04	6.79	3.6	19.3
51	DIAZOL		$C_6H_2N_4O_5$	4.23	4.23	7	7.21	-3.1	22.2
52	HNDS		$C_{12}H_4N_6O_{12}S$	4.15	4.36	7	7.31	-4.5	23.9

Table 3 (Continued)

Serial number	Compound	Structure	Empirical formula	Detonation factor		Velocity of detonation (km/s)		Error (%)	C-J pressure (GPa)
				Reported	LOTUSES	Experimental	LOTUSES		
53	TNT		C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	3.93	3.92	6.9	6.66	3.4	19.2
54	NM/TNM	and	CH <sub>2.4</sub> N <sub>1.6</sub> O <sub>3.2</sub>	4.20	4.50	6.88	7.70	-8.9	22.4
55	TNC		C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	4.00	3.93	6.85	6.66	2.7	19.4
56	DNPEN		C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>8</sub>	3.83	3.82	6.8	6.48	4.7	17.7
57	ET PIC		C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>7</sub>	3.73	3.73	6.5	6.30	3.0	16.3
58	TNAN		C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>7</sub>	4.00	4.00	6.8	6.80	0.0	19.6
59	DEGN		C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	3.97	3.97	6.76	6.74	0.3	16.96
60	TNM		CN <sub>4</sub> O <sub>8</sub>	3.97	3.97	6.55	6.75	-3.0	19.5
61	TMPTN		C <sub>6</sub> H <sub>8</sub> N <sub>3</sub> O <sub>9</sub>	4.01	4.01	6.44	6.82	-5.8	18.6
62	DNPF	Dinitropropylfumarate	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>12</sub>	3.74	4.08	6.38	6.94	-8.8	20.3
63	TNN		C <sub>10</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	3.39	3.4	6	5.69	5.2	19.9

Abbreviations used in Table 3

Serial number	Compound	Chemical name	Serial number	Compound	Chemical name
1	HNB	Hexanitrobenzene	33	HNAB	Hexanitroazobenzene
2	SORGUYL	Tetranitroglycouril	34	PETRIN	Pentaerythritol trinitrate
3	HMX	Cyclotetramethylene tetranitramine	35	DNPTB	Dinitropropyltrinitrobutyrate
4	BTNEU	Bis-trinitroethylurea	36	TNPN	Trinitrophenoxy ethylnitrate
5	9404	HMX + NC + chloroethyl phosphate	37	DPEHN	Dipentaerythritolhexanitrate
6	RDX	Cyclotrimethylene trinitramine	38	PIC ACID	Trinitrophenol
7	BTNEN	Bis-trinitroethylnitramine	39	DIPAM	Hexanitrobiphenyldiamine
8	HN	Hydrazine mononitrate	40	TNA	Trinitroaniline
9	BFT	Benzotrifuroxan	41	XPL D	Ammonium picrate
10	908	HMX-estane	42	GTNB	Ethyleneglycol di-trinitrobutyrate
8	OCTOL	HMX + TNT	43	EGDN	Ethyleneglycoldinitrate
12	9010	RDX + Kel-F	44	TNB	Trinitrobenzene
13	CYCLOTOL	RDX-TNT	45	TACOT	Tetranitrodibenzo-tetrazapentalene
14	9205	RDX-polystyrene-ethylhexylphosphate	46	HNDP	Hexanitrodiphenylamine
15	TNETB	Triethyltrinitrobutyrate	47	HNDPO	Hexanitrodiphenyloxide
16	PETN	Pentaerythritol tetranitrate	48	HNS	Hexanitrostilbene
17	MHN	Mannitol hexanitrate	49	DNDMOA	Dinitrodimethylloxamide
18	EDNA	Ethylenedinitramine	50	FIVONITE	Tetramethylolcyclo-pentanone
19	NQ	Nitroguanidine	51	DIAZ	Diazodinitrophenol
20	DINGU	Dinitroglycouril	52	HNDS	Hexanitrodiphenylsulfide
21	DNP	Bis-dinitropropyl nitramine	53	TNT	Trinitrotoluene
22	COMP B-3	RDX-TNT	54	NM/TNM	Nitromethane/Tetranitromethane
23	COMP C-4	RDX-polyisobutylene	55	TNC	Trinitrocresol
24	DINA	Dioxyethylnitraminedinitrate	56	DNPEN	Dinitrophenoxyethyl nitrate
25	TATB	Triaminotrinitrobenzene	57	ET PIC	Ethylpicrate
26	TETRYL	Trinitrophenylmethyl nitramine	58	TNAN	Trinitroanisole
27	NIBTN	Nitroisobutyltrinitrate	59	DEGN	Diethyleneglycol dinitrate
28	R-SALT	Cyclotrimethylenetrinitrosamine	60	TNM	Tetranitromethane
29	TPEON	Tri-pentaerythritol octanitrate	61	TMPTN	Trimethyl ethylmethane trinitrate
30	NG	Nitroglycerin	62	DNPF	Dinitropropyl fumarate
31	EDD	Ethylenediaminedinitrate	63	TNN	Trinitronaphthalene
32	DATB	Diaminotrinitrobenzene			

The theoretically predicted performance parameters obtained from LOTUSES give a fair idea to the HEMs scientists and technologists about the performance level of the unknown HEMs in comparison to bench mark known explosives before embarking upon its synthesis and evaluation. The LOTUSES code does not calculate performance parameters of energetic co-ordination compounds.

The density, velocity of detonation, C–J pressure, heat of explosion, and power index predicted in this work will be of great value in envisaging the risks associated with an accidental explosion/detonation. In general, HEMs having higher density will have higher detonation factor, detonation velocity, C–J pressure, heat of explosion and power index. All these parameters are depend on each other. In general, most of the HEMs studied for the theoretical performance

prediction under the present study fall under hazard division 1.1 and 1.2. According to UN International system of classification, the hazard division 1.1 is assigned to the HEMs having potential of blast, high velocity shattering effects as well as low velocity explosion in the event of accidental initiation. Accidental initiation of the secondary explosives may lead to severe structural damage and resulting in burning followed by exploding a few at a time. In case if the predicted HEMs undergo accidental initiation resulting in burning and exploding progressively, a few at a time falls under the UN classification hazard division 1.2. In this case blast effects are limited to the immediate vicinity. Accordingly depending upon the assigned hazard class to the theoretically predicted HEMs, safety care must exercised before embarking upon their synthesis, scale up,

Table 4  
Comparison of predicated (by LOTUSES) and experimentally observed thermodynamic parameters

Serial number	HEMs name	Empirical formula	Enthalpy of formation (kcal/kg)	Heat of explosion (kJ/kg)			Volume of detonation gases (l/kg)			Power index (%)
				Experimental	LOTUSES	Error (%)	Experimental	LOTUSES	Error (%)	
1	Bi-trinitroethyl nitramine (BTENA)	C <sub>5</sub> H <sub>5</sub> N <sub>8</sub> O <sub>14</sub>	−197.6	4857	5287.4	−8.9	705	736.3	−4.4	144.1
2	Hexanitroethane HNE	C <sub>2</sub> N <sub>6</sub> O <sub>12</sub>	95.3	3102	3023.2	2.5	672	708.7	−5.5	79.3
3	Tetranitromethane (TNM)	CN <sub>4</sub> O <sub>8</sub>	44.9	2259	2196.4	2.8	685	723.2	−5.6	58.8
4	Bitrinitroethylurea (BTNEU)	C <sub>5</sub> H <sub>6</sub> N <sub>8</sub> O <sub>13</sub>	−199.2	6542	6144.7	6.1	768	734.2	4.4	167.1
5	Nitroisobutylglycerol trinitrate (NIBTN)	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	−190.8	7755	7243.7	6.6	801	743.3	7.2	199.4
6	Mannitolhexa nitrate (MHN)	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>18</sub>	−340.6	6380	5940.4	6.9	755	731.6	3.1	160.9
7	Nitrocellulose	C <sub>12</sub> H <sub>14</sub> N <sub>6</sub> O <sub>22</sub>	−593.6	4408	4047.5	8.2	875	874.8	0.0	131.1
8	Ethylene glycoldinitrate EGDN	C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>6</sub>	−383.2	7390	6757.9	8.6	816	776.9	4.8	194.4
9	PETN	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub>	−402.4	6404	5821.7	9.1	823	822.2	0.1	177.2
10	Methyl nitrate	CH <sub>3</sub> NO <sub>3</sub>	−483.1	6869	6230.6	9.3	909	920.2	−1.2	212.3
8	Butene triol trinitrate	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O <sub>9</sub>	−403.4	6153	5516.2	10.4	865	882.0	−1.9	180.1
12	RDX	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	76.1	5723	5096.3	10.9	900	957.4	−6.4	180.7
13	Dinitronaphthalene	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	67.4	2635	2331.7	8.5	837	861.0	−2.9	74.8
14	Nitrourea	CH <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	−639.7	3865	3374.7	12.7	853	899.7	−5.5	82.4
15	PVN	C <sub>2</sub> H <sub>3</sub> NO <sub>3</sub>	−298.6	4574	3978.7	13.0	1009	1061.4	−5.2	156.4
16	PETRIN	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> O <sub>10</sub>	−494.2	5301	4603.4	13.2	918	958.6	−4.4	163.4
17	DIPEHN	C <sub>10</sub> H <sub>16</sub> N <sub>6</sub> O <sub>19</sub>	−446	5208	4496.5	13.7	907	946.5	−4.3	157.6
18	DINA	C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>8</sub>	−314	5384	4579.1	14.9	943	984	−4.3	166.8
19	Nitroglycerine	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub>	−392	6766	5692.7	15.9	782	780.4	0.2	164.5
20	Diethylene glycol dinitrate	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	−528	4522	3772.5	16.6	1030	1084.4	−5.3	151.5

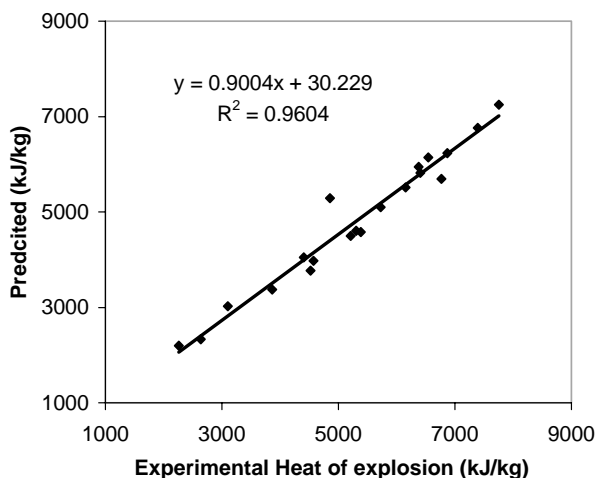


Fig. 6. Experimental vs. predicted heat of explosion.

processing/evaluation, storage, transport and use as per the UN classification of hazards category.

### 3.2. Thermodynamic parameters of HEMs

The methodology assumes that the heat of explosion of high energy compounds can be approximated as the difference between the heat formation of the detonation products and that of the explosives. The decomposition gases are assumed to comprise almost solely of CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, O<sub>2</sub>, and N<sub>2</sub>. The experimentally determined values and the predicted heat of explosion as well as volume of detonation gases with power index of high energetic materials are presented (Table 4) and plotted as graph in Figs. 6 and 7. For all data points, linear regression analysis of experimental and predicted heat of explosion yields the correlation coefficient  $R^2 = 0.9604$  with a linear equation  $y = 0.90x - 30.0$ . Bar diagrams represented in Figs. 8 and 9 reflect the error analysis on deviation between the predicted and experimentally determined heat of explosion and volume of detonation gases, respectively. The linear regression analysis of volume of detonation product gases yields the correlation coefficient

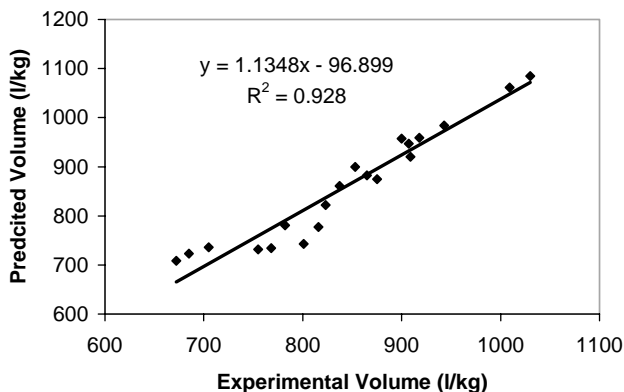


Fig. 7. Experimental vs. predicted volume of explosion products.

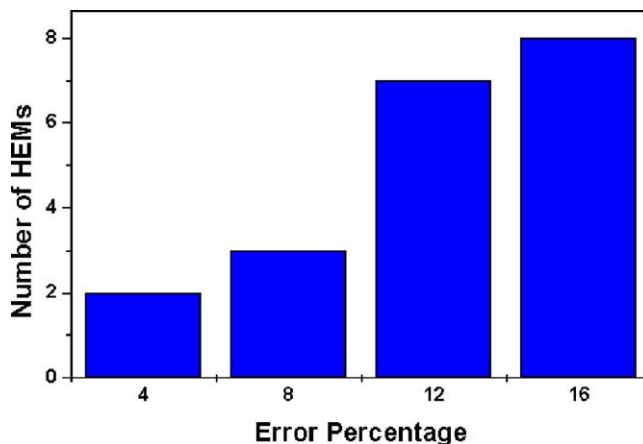


Fig. 8. Error percentage in prediction of heat of explosion vs. number of HEMs.

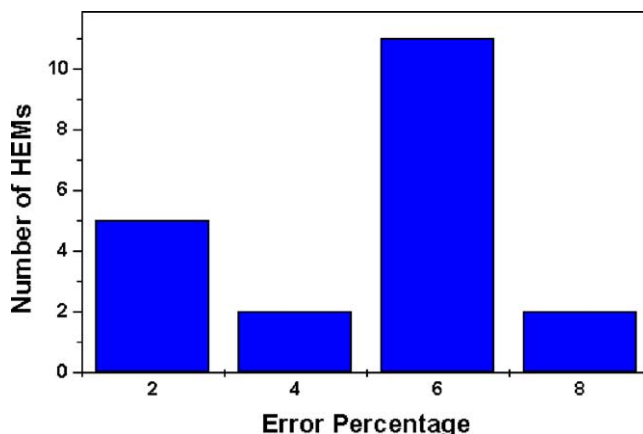


Fig. 9. Error percentage in prediction of volume of detonation gases vs. number of HEMs.

$R^2 = 0.93$  with a linear equation  $y = 1.138x - 96.9$ . These linear coefficient values reveal that the predicted values by LOTUSES are in agreement with the experimentally determined values.

## 4. Conclusion

The present paper reports the newly developed user friendly code named LOTUSES for the theoretical performance prediction of parameters such as density, decomposition products, detonation factor ( $F$ ), VOD, and  $P_{c_j}$  for wide range of explosives. The linear regression coefficient  $R^2 = 0.83$  and  $0.91$  are obtained for experimental versus predicted density and velocity of detonation. It reflects that the predicted values are close to experimentally determined velocity of detonation as reported in literature to great extent. The calculations presented herein show that this computational code predicts the heats of detonation of explosive materials in rapid assessment and screening of notional energetic materials. The predicted detonation



parameters bring out that most of the HEMs studied during this work fall under UN hazard division 1.1 and 1.2. Therefore, adequate safety measures need to be exercised during handling. Finally, it is concluded that the computational methodology for thermodynamic analysis of high energy materials will allow theoretical screening of notional materials for identification of promising candidates for additional study and elimination of weaker candidates from further consideration. Thereby, reducing cost associated with the development programme of the materials. The calculation of explosive parameters based on thermodynamic concepts is fast and simple. The theoretically predicted properties by LOTUSES can be directly printed as well as stored in various formats (.txt, .htm, .doc, .pdf) and can be heard in Audio format through multimedia speakers.

### Acknowledgements

Authors are highly grateful to Shri AS Rajagopal, Director, Armament Research & Development Establishment, Pashan, Pune and Dr. Haridwar Singh, Director, High Energy Material Research Laboratory, Pune for providing infrastructure and permission to carry out this work and present this paper. Authors express their deep sense of gratitude to Shri S.R. Madhavan, Scientist 'E', OSD-to-Director, ARDE for his inspiration and constant motivation. We record our thanks to Staffs and Officers of TIRC of both ARDE and HEMRL for literature survey through various technical resources.

### References

- [1] J.R. Stine, Prediction of crystal densities of organic explosives by group additivity, Los Alamos National Laboratory's Report, New Mexico, 1981.
- [2] T.S. Pivina, D.V. Sukhachev, A.V. Evtushenko, L.I. Khmel'nitskii, *Propel. Explos. Pyrotechn.* 20 (1995) 5.
- [3] D.S. Chen, D.S. Wong, *Propel. Explos. Pyrotechn.* 23 (1998) 296.
- [4] T.S. Pivina, V.V. Shcherbukhin, M.S. Molchanova, N.S. Zefirov, *Propel. Explos. Pyrotechn.* 20 (1995) 144.
- [5] D.R. Forshey, J.C. Cooper, W.J. Doyak, *Explosivstoffe* 6 (1969) 125.
- [6] P.A. Persson, TIGER WIN—a window PC code for computing explosive performance and thermodynamic properties, in: Proceedings of 2000 High-tech Seminar, State-of-the Art Blasting Technology and Explosive Applications, 2000, p. 541.
- [7] J. Akhavan, *The Chemistry of Explosives*, The Royal Society of Chemistry, UK, 1998.
- [8] L.R. Rothstein, R. Petersen, *Propel. Explos. Pyrotechn.* 4 (1979) 56.
- [9] P.W. Cooper, Extending estimation of C–J pressure of explosives to the very low-density region, in: Proceedings of the 18th International Pyrotechnic Symposium, Breckenridge, CO, 1992.
- [10] W. Fickett, W.C. Davis, *Detonation*, University of California Press, Berkeley, 1979.
- [11] R. Meyer, *Explosives*, second ed., Verlag Chemie, Germany, 1981.
- [12] L.R. Rothstein, *Propel. Explos. Pyrotechn.* 6 (1981) 91.
- [13] M.J. Kamlet, J.E. Abland, *J. Chem. Phys.* 48 (1968) 23.
- [14] M.J. Kamlet, J.E. Abland, *J. Chem. Phys.* 48 (1968) 36.
- [15] M.J. Kamlet, J.E. Abland, *J. Chem. Phys.* 48 (1968) 43.
- [16] M.J. Kamlet, J.E. Abland, *J. Chem. Phys.* 48 (1968) 3685.
- [17] M.J. Kamlet, J.E. Abland, *Combust. Flame* 38 (1980) 221.
- [18] S.W. Benson, J.H. Buss, *J. Chem. Phys.* 29 (1958) 546.
- [19] B.M. Rice, J. Hare, *Thermochim. Acta* 384 (2002) 377.