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Prediction of Detonation Velocity and N–O Composition of High Energy C–H–N–O Explosives by Means of Artificial Neural Networks

Nichith Chandrasekaran,*[a] Charlie Oommen,[a] V. R. Sanal Kumar,[b] Alexander N. Lukin,[c] Victor S. Abrukov,[d] and Darya A. Anufrieva[d]

Abstract: The possibilities of the application of Data Science Methods in predicting certain macroscopic properties have been examined in energetic compounds. Artificial neural networks, one of the most promising methods of Data Science, has been used for predicting detonation velocity based on a trained set comprising of a large data set containing 104 data points extracted from over 65 explosive compounds and compositions with diverse characteristics and properties. The utility of the method has been demonstrated through validation for over 37 explosive compounds again with diverse characteristics constituting to a data set of 74 data points. The usefulness and versatility of the method is clear as it exhibits similar predictive accuracy on comparison with the similar data derived from two other well-known empirical models. Such predictive capabilities will be a great tool for engineers and scientists working with high energetic explosives for quick and simple prediction of detonation velocity given the chemical composition and vice versa.

Keywords: Detonation velocity · High energetic materials · Data science · Artificial neural networks · Multifactor computational models · Knowledge Base Formatting

1 Introduction

Among the chemists, engineers and scientists dealing with explosives, there is always a need and consequently a search for new explosives with improved properties. The important properties of explosives include performance parameters, sensitivity parameters and physical parameters. Among the different parameters, detonation velocity (D) is one of the basic indicator of performance of explosives and is related to the fundamental elemental and structural properties of the explosives. Prediction of such properties is of great interest to those dealing with synthesis of explosives. Such calculations or predictions of properties of explosives could be helpful in deciding the potential of a new explosive. Theoretical determination of detonation properties are done using hydrodynamic theory with the help of equations of state for detonation products. Some widely used equation of state are Becker-Kistiakowsky-Wilson equation of state [1], Jacobs-Cowperthwaite-Zwisler equation of state [2] and Kihara-Hikita-Tanaka equation of state [3]. There are also some computer codes like RUBY [4] and TIGER [5] which compute the explosive properties with the help of hydrodynamic theory and the equation of state. But these models and codes are very complex. It is hence desirable to have methods/models to predict detonation properties without the need for detailed training in calculation using thermodynamic and hydrodynamic equations.

Simpler empirical methods like Kamlet and Jacob, Rothstein and Petersen etc., can give a prediction which is of similar accuracy to that of the computer code simulated properties. Kamlet and Jacob method [6] shows simple relationship to calculate the detonation velocity (D) at loading densities above 1 g cm^{-3}. The equations imply that the dependence of detonation velocity is only on chemical energy of detonation reaction (Q), number of moles of detonation gases per unit weight of explosive (N), average molecular weight of the gases (M), and loading density (ρ_0). N, M and Q estimation is based on the use of the H_2O–CO_2 arbitrary decomposition scheme.

[a] *N. Chandrasekaran, C. Oommen*
Energetic Materials Research Lab – Department of Aerospace Engineering
Indian Institute of Science, Bengaluru 560012, India
**e-mail: nichith@gmail.com*
[b] *V. R. S. Kumar*
Department of Aeronautical Engineering
Kumaraguru College of Technology, Coimbatore 641049, India
[c] *A. N. Lukin*
Western-Caucasus Research Center, Tuapse 352808, Russia
[d] *V. S. Abrukov, D. A. Anufrieva*
Department of Applied Physics and Nanotechnology
Chuvash State University, Cheboksary 428010, Russia

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$$D = A\Phi^{1/2}(1 + B\rho_0) \quad (1)$$

$$\Phi = NM^{1/2}Q^{1/2} \quad (2)$$

$$N = \frac{2c + 2d + b}{48a + 4b + 56c + 64d} \quad (3)$$

$$M = \frac{56c - 88d - 8b}{2c + 2d + b} \quad (4)$$

$$Q = \frac{28.9b + 47.0(d - \frac{1}{2}b) + \Delta H_f(explosive)}{12a + b + 14c + 16d} \quad (5)$$

a, *b*, *c* and *d* are the elemental compositions of carbon, hydrogen, nitrogen and oxygen respectively. ΔH_f is the heat of formation of the explosive in kcal/mol. Rothstein and Petersen [7] method predicts D of explosives at their theoretical maximum density (TMD). The empirical relation is given by the following equations:

$$D' = D_0 + (\rho_{TMD} - \rho_0) \times 3 \quad (6)$$

$$D' = \frac{F - 0.26}{0.55} \quad (7)$$

$$F = \left[100 \times \frac{n(O) + n(N) - \frac{n(H)}{2n(O)} + \frac{A}{3} - \frac{n(B)}{1.75} - \frac{n(C)}{2.5} - \frac{n(D)}{4} - \frac{n(E)}{5}}{MW}\right] - G \quad (8)$$

D′ is the detonation velocity at the ρ_{TMD} (theoretical maximum density) and D_0 is the detonation velocity at a loading density ρ_0. The factor F is expressed as an empirical relation of the following parameters: G = 0 or 0.4 (for liquid explosives and solid explosives respectively); A = 1 and 0 (for aromatic compounds or otherwise respectively); MW is the molecular weight; *n*(O), *n*(N) and *n*(H) are the number of oxygen, nitrogen and hydrogen atoms respectively; *n*(B) is the number of oxygen atoms in excess of those already available to form CO_2 and H_2O; *n*(C) is number of oxygen atoms doubly bonded directly to carbon as in C=O; *n*(D) is number of oxygen atoms singly bonded directly to carbon as in C–O–R linkage where R can equal –H, $-NH_4$, –C, etc.; and *n*(E) is number of nitrato groups existing either as nitrate-esters or as a nitrate salts. Jain [8] showed that properties of explosives could be correlated using their oxidation and reduction valences. More recent studies on prediction of detonation velocity has been done for both CHNO explosives, CHNFOCl and aluminized explosives [9–11]. Keshavarz [9] gives an empirical relation for predicting detonation velocity for CHNOF and aluminized explosives at maximum nominal density. The relation is given by

$$D' = D'_{core} + 0.996D'_{In} - 0.741D'_{De} \quad (9)$$

$$D'_{core} = 7.03 - 0.162a - 0.0206b + 0.228c + 0.0714d \quad (10)$$

Here D' and D'_{core} are expressed in km/s; a, b, c and d are the number of moles of C, H, N and O atoms respectively; D'_{In} and D'_{De} are two correcting functions that increase and decrease the predicted results on the basis of D'_{core} by taking into account fluorine and aluminum content. This was shown to predict the detonation velocity better than the RP method. Similarly another empirical relation was developed by Keshavarz et. al [10] for predicting the detonation velocity of CHNOFCl and aluminized explosives at any loading densities which is given by

$$D = 1.412n_g^{0.5}\left(\overline{M}_g Q\right)^{0.25}\rho_0 + 2.00 \quad (11)$$

Where D is the detonation velocity in km/s, n_g is the number of moles of gaseous products of detonation per gram of explosive, $\overline{M}_g$ is the average molecular weight of the gaseous products and ρ_0 is the loading density. This has been shown to have very good predicting capabilities on par with K-J method with good predicting capability at lower loading densities too.

By studying these empirical relations, we can understand that detonation velocity prediction with good accuracy can be made with a model using the composition and structure of explosives, heat of formation of explosive and loading density. So a model with only C–H–N–O (i.e., chemical composition) along with heat of formation of the explosive and loading density as inputs is desirable as it would be simple and also have good predictive nature. It is also very useful if an inverse prediction capability of predicting the chemical composition for a decided detonation velocity can be made effortlessly.

With these requirements, it is easy for one to see that data science methods like the artificial neural network (ANN) can be a very viable option to develop such predictive capabilities because of their ability to be multifactor models which can establish dependencies between all the variables. Possibility of using data science methods is facilitated as experimental data of detonation properties for a large number of explosives is available in literature [12–17].

In the recent years ANN technique has been used for prediction of impact sensitivity of high energetic materials [18–22]. Besides, other machine learning techniques also have been used for prediction of properties of high energetic materials from their molecular structure [23]

An approach to use ANN technique to predict the detonation velocity had been previously attempted by Chen et al. [24]. But in their model they have considered only chemical composition of C–H–N–O for predicting detonation velocity. They had concluded that their model cannot be accurate in predicting properties of isomers since only stoichiometric numbers of chemical composition are used as inputs. Besides, they have limited inputs with critical parameters like loading density and heat of formation missing in the inputs. It can be noted from Kamlet and Hur-

witz [6] and experimental data from literature [12–17] that loading density also influences detonation velocity.

It would be interesting if a model can predict the compositions to get a necessary detonation velocity. But such an inverse mapping model had not been attempted hitherto in literature pertaining to explosives.

A better generalized and versatile ANN model to overcome the limitations of [24] should incorporate the variation of detonation velocity with loading density along with chemical composition and some property of the explosive that could be different for isomers as inputs. Hence this work attempts to come up with simple and accurate back propagating feed forward neural networks which can be used for a direct problem such as predicting detonation velocity from chemical composition, loading density etc. and an inverse problem such as predicting the composition for a given detonation velocity.

2 Artificial Neural Networks Technique and Modelling

2.1 ANN Technique

The ANN can be considered as a universal tool for multidimensional approximation. The theoretical details of ANN can be found elsewhere [25]. The ANN technique used here is the same as given in [26]. Each elementary neuron shown in Figure 1 executes the following operations:

$$S = \sum_{i=1}^{n} X_i W_i \tag{12}$$

$$Y = f(S) \tag{13}$$

$$f(S) = \frac{1}{1 + e^{-\alpha S}} \tag{14}$$

Where W_i is the weight between neurons; S is the result of summation; X_i is the component of input; Y is the output of each neuron; n is the number of inputs of a neuron; f is the non-linear transformation or activation function; and α is the steepness factor.

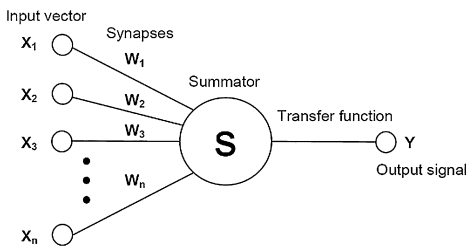

Figure 1. Scheme of an elementary neuron.

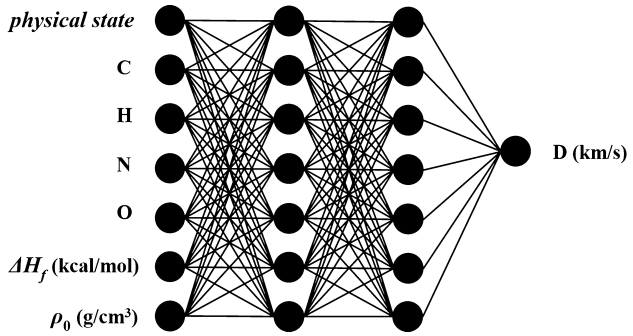

Figure 2. Schematic of ANN model 1.

2.2 Modeling

The analytical platform, Loginom [27], used for creating and operating the model was developed by Base Group Labs. We have used a feed forward neural network. This paper deals with two problems, 1) Direct problem 2) Indirect problem.

We have considered the direct problem as one in which the chemical composition and properties of explosives are given as inputs and the detonation velocity is predicted. This is given by the ANN model 1 and is shown in Figure 2.

It consists of 1 input layer consisting of 7 neurons for the seven input variables namely, the elemental composition of C, H, N and O in the compound, loading density, physical state and heat of formation of the explosive. There are 2 hidden layers each consisting of 7 neurons and the output layer consists of 1 neuron which gives the detonation velocity as output. The reasons for coming up with this set of input variables are as follows. Using physical state can help differentiate between solid and liquid explosives as in some cases both solid and liquid phases can exist (for example TNT and liquid TNT). In such cases just the stoichiometry and loading density may not be enough to differentiate between them as we would end up with the same detonation velocity prediction. Heat of formation of the explosive is a property that appears in most of the empirical methods for predicting D and additionally it is useful in differentiating between explosives having the same elemental composition (isomers). Hence we have included it as one of the inputs. The dataset used to train this model is given in table S1 in the supplementary file. It consists of 104 data points for a wide range of CHNO explosives (liquid and solid explosives; pure and mixtures) at different loading densities. These data points were compiled using experimental data available in literature [12–17].

The inverse problem considered here is to predict a suitable elemental composition of N and O in a CHNO explosive composition for a given detonation velocity, material properties and C and H composition. This is done by the ANN model 2 shown in Figure 3. Here we have considered 1 input layer with 5 neurons for the input variables of ele-

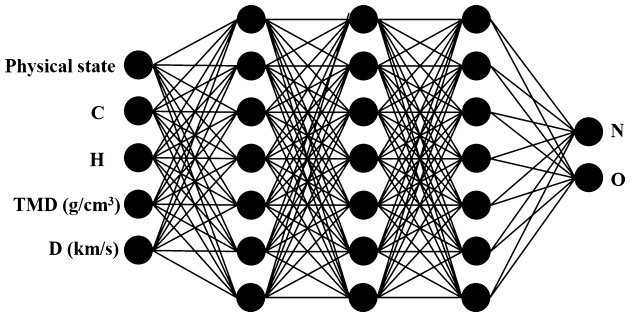

Figure 3. Schematic of ANN model 2.

mental composition of C and H, theoretical maximum density (TMD), physical state and detonation velocity. Here TMD was chosen as input because it was indicated that the detonation velocity is a characteristic of individual explosive and is not influenced by external factors if density of the explosive is at its maximum value [9, 14]. Hence it would be a suitable input parameter when we are predicting the composition of an explosive with detonation velocity as one of the inputs. There are 3 hidden layers consisting of 7 neurons each and 1 output layer with 2 neurons giving the composition of N and O as output. The training dataset used to train this model consists of experimental data of explosives taken from [12–17]. 45 data points were used to train and 9 data points were used to validate. The dataset used to train is given in table S2 in the supplementary file. The data set consists of only pure explosive (both liquid and solid) at their theoretical maximum density.

The number of hidden layers and number of neurons in the hidden layer are important for the performance and accuracy of the model. It is known that too few neurons can result in under-fitting and too many would result in over-fitting. There is no clear rule for determining the optimal number of hidden layer neurons. In both the models, we started with lesser neurons and more neurons were added until the required accuracy was reached. Similar approach was followed in the selection of number of hidden layers. The models were optimized by tuning the weights using the backpropagation algorithm. In both cases, a sigmoid transfer function with slope steepness factor of 1 was used for the training procedure.

3 Results and Discussion

3.1 Calculation of Detonation Velocity (D): Direct Problem

ANN model 1 was trained by data from a set of explosives selected from a diverse range of explosives with different structural and compositional features. The details of the training data set is given in Table S1. The scatter graph of the training set for a range of detonation velocity is shown in Figure 4. Since the preliminary validation was found

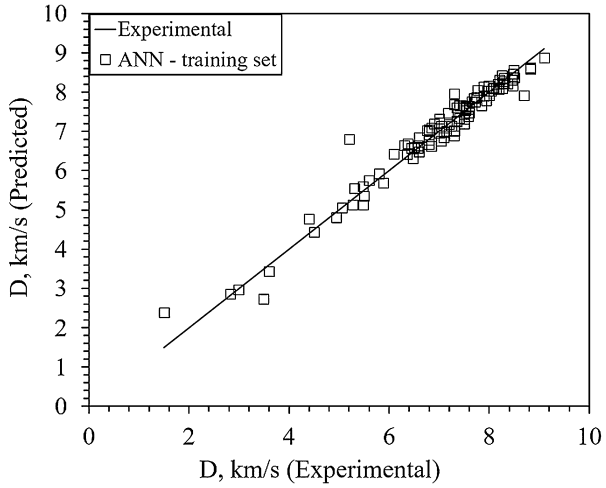

Figure 4. Scatter graph of the training set showing the detonation velocity predicted by ANN vs Experimental D

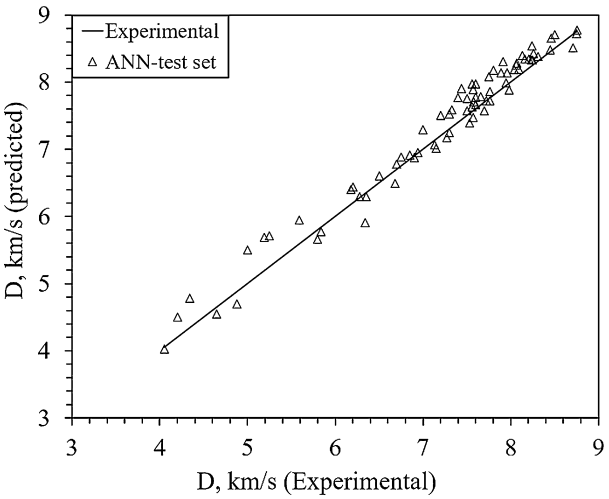

Figure 5. Scatter graph of the test set showing the detonation velocity predicted by ANN vs Experimental D

promising based on the scatter graph, the same model was further validated by predicting the detonation velocity for a set of another 37 explosives at different loading densities giving a total of 74 data points. This is shown in Figure 5 as the scatter graph. The graph shows the values of detonation velocity predicted by the ANN model in comparison with experimental detonation velocities. The correlation coefficient for Figure 4 and Figure 5 are 0.978 and 0.985 respectively. The correlation coefficient r is given by

$$r = \frac{m(\sum xy) - (\sum x)(\sum y)}{\sqrt{m(\sum x^2) - (\sum x)^2}\sqrt{m(\sum y^2) - (\sum y)^2}} \quad (15)$$

where m is the number of data points. Table 1 gives the

Table 1. Comparison of predicted detonation velocity D by ANN, the Keshavarz method [10] and KJ method [6] at different loading density with experimental data for CHNO explosives; ΔH_f in kJ mol^{-1}; ρ_0 in g cm^{-3}; all D data in km s^{-1} (Direct problem).

No	Name (Phy. State)	Molecular formula	ΔH_f	ρ_0	D_{exp}	D_{ANN}	%Dev	D_{Kesh}	%Dev	D_{KJ}	%Dev
1	ABH (s)	$C_{24}H_6N_{14}O_{24}$	485.34	1.78	7.60[f]	7.775	*2.30*	7.99	*5.18*	7.69	*1.18*
				1.64	7.20[g]	7.505	*4.24*	7.53	*4.52*	7.27	*0.97*
2	BTF (s)	$C_6N_6O_6$	605	1.76	8.26[g]	8.425	*2.00*	8.31	*0.56*	8.05	*−2.54*
3	Cyclotol 50/50 (s)	$C_{2.22}H_{2.45}N_{2.01}O_{2.67}$	0.04	1.63	7.66[g]	7.781	*1.58*	7.66	*0.00*	7.59	*−0.91*
4	Cyclotol 60/40 (s)	$C_{2.04}H_{2.5}N_{2.15}O_{2.68}$	4.81	1.74	8.09[g]	8.195	*1.30*	8.14	*0.57*	8.07	*−0.25*
				1.72	7.89[g]	8.142	*3.19*	8.07	*2.23*	8.00	*1.27*
5	Cyclotol 65/35 (s)	$C_{1.96}H_{2.53}N_{2.22}O_{2.68}$	8.33	1.72	8.04[g]	8.184	*1.79*	8.11	*0.85*	8.07	*0.37*
6	Cyclotol 70/30 (s)	$C_{1.87}H_{2.56}N_{2.29}O_{2.68}$	11.13	1.73	8.06[g]	8.251	*2.37*	8.19	*1.57*	8.17	*1.36*
7	Cyclotol 75/25 (s)	$C_{1.78}H_{2.58}N_{2.36}O_{2.69}$	13.4	1.62	7.95[g]	7.985	*0.44*	7.84	*−1.45*	7.87	*−1.01*
8	Cyclotol 77/23 (s)	$C_{1.75}H_{2.59}N_{2.38}O_{2.69}$	14.98	1.74	8.25[g]	8.327	*0.93*	8.28	*0.37*	8.29	*0.48*
9	Cyclotol 78/22 (s)	$C_{1.73}H_{2.59}N_{2.4}O_{2.69}$	15.52	1.76	8.31[g]	8.381	*0.85*	8.36	*0.58*	8.37	*0.72*
10	DATB (s)	$C_6H_5N_5O_6$	−98.70	1.8	7.60[g]	7.66	*0.79*	7.65	*0.63*	7.60	*0.00*
11	DIPAM (s)	$C_{12}H_6N_8O_{12}$	−28.45	1.79	7.50[f]	7.753	*3.37*	7.81	*4.20*	7.62	*1.60*
12	EDC-11 (s)	$C_{1.986}H_{2.78}N_{2.23}O_{2.63}$	4.52	1.78	8.21[f]	8.34	*1.58*	8.30	*1.10*	8.24	*0.37*
13	EDC-24 (s)	$C_{1.64}H_{3.29}N_{2.57}O_{2.57}$	18.28	1.78	8.71[f]	8.508	*−2.32*	8.50	*−2.41*	8.49	*−2.53*
14	EDNA (s)	$C_2H_6N_4O_4$	−103.81	1.663	8.24[a]	8.33	*1.13*	–	–	8.127	*−1.37*
				1.56	7.75[a]	8.08	*4.26*	–	–	7.789	*0.50*
				1.49	7.57[a]	7.89	*4.23*	–	–	7.547	*−0.30*
15	EGDN (l)	$C_2H_4N_2O_6$	–242.84	1.48	7.30[e]	7.25	*–0.68*	–	–	–	–
16	EXP D (s)	$C_6H_6N_4O_7$	−386.39	1.6	7.15[e]	7.015	*1.18*	–	–	–	–
				1.55	6.85[g]	6.917	*0.98*	6.72	*−1.84*	6.8	*−0.73*
				1.48	6.70[f]	6.779	*−1.89*	6.51	*−2.80*	6.60	*−1.49*
17	HMX (s)	$C_4H_8N_8O_8$	75.02	1.77	8.50[a]	8.709	*2.46*	–	–	8.671	*2.01*
				1.6	7.91[g]	8.303	*4.97*	7.92	*0.09*	8.09	*2.28*
				1.4	7.30[g]	7.523	*3.05*	7.18	*−1.60*	7.41	*1.51*
				1.00	5.80[g]	5.658	*−2.45*	5.72	*−1.47*	6.04	*4.14*
				0.75	4.88[g]	4.697	*−3.75*	4.80	*−1.69*	5.19	*6.35*
18	HNS (s)	$C_{14}H_6N_6O_{12}$	78.20	1.74	7.13[f]	7.065	*–0.91*	7.69	*7.80*	7.47	*4.83*
19	NG (l)	$C_3H_5N_3O_9$	−371	1.6	7.70[g]	7.575	*−1.62*	7.93	*2.92*	8.17	*6.08*
20	NM (l)	CH_3NO_2	−113	1.13	6.28[f]	6.295	*0.24*	6.14	*−2.28*	6.38	*1.59*
				1.13	6.35[g]	6.295	*−0.87*	6.14	*−3.6*	6.38	*0.47*
21	NONA (s)	$C_{18}H_5N_9O_{18}$	114.64	1.78	7.56[f]	7.97	*5.42*	–	–	–	–
				1.70	7.40[g]	7.77	*5.00*	–	–	–	–
22	Toluene/NM (14.5/85.5) (l)	$C_{2.503}H_{5.461}N_{1.4006}O_{2.8013}$	−160.71	1.09	5.84[f]	5.772	*−1.16*	5.49	*−6.00*	5.79	*0.86*
23	NQ (s)	$CH_4N_4O_2$	−92.5	1.63	7.98[g]	7.882	*−1.23*	7.29	*−8.64*	7.40	*−7.27*
24	Octol 76/23 (s)	$C_{1.76}H_{2.58}N_{2.37}O_{2.69}$	12.76	1.81	8.45[g]	8.476	*0.31*	8.52	*0.82*	8.51	*0.71*
25	Octol 60/40 (s)	$C_{2.04}H_{2.5}N_{2.15}O_{2.68}$	4.14	1.8	8.16[g]	8.344	*2.25*	8.34	*2.25*	8.26	*1.23*
26	ONT (s)	$C_{18}H_6N_8O_{16}$	82.72	1.8	7.33[h]	7.589	*3.53*	–	–	–	–
27	PBXC-116 (s)	$C_{1.968}H_{3.7463}N_{2.356}O_{2.4744}$	4.52	1.65	7.96[f]	8.141	*2.27*	7.86	*−1.22*	7.54	*−5.28*
28	PBXC-119 (s)	$C_{1.817}H_{4.1073}N_{2.2149}O_{2.688}$	18.28	1.64	8.07[f]	8.284	*2.65*	8.14	*0.91*	7.92	*−1.86*
29	Pentolite 50/50 (s)	$C_{2.33}H_{2.37}N_{1.29}O_{3.22}$	−100	1.64	7.53[g]	7.39	*−1.86*	7.67	*1.90*	7.62	*1.20*
30	Picric acid (s)	$C_6H_3N_3O_7$	−214.60	1.76	7.57[g]	7.477	*−1.23*	7.69	*1.58*	7.55	*−0.24*
31	RDX (s)	$C_3H_6N_6O_6$	61.55	1.8	8.75[f]	8.774	*0.23*	8.67	*−0.95*	8.79	*0.46*
				1.76	8.75[e]	8.719	*−0.35*	–	–	–	–
				1.72	8.46[g]	8.653	*2.28*	8.37	*−1.04*	8.51	*0.59*
				1.66	8.24[g]	8.537	*3.60*	8.15	*−1.07*	8.31	*0.85*
				1.6	8.13[g]	8.396	*3.27*	7.93	*−2.45*	8.10	*−0.37*
				1.46	7.60[g]	7.972	*4.89*	7.42	*−2.42*	7.62	*0.26*
				1.44	7.44[a]	7.901	*6.20*	–	–	7.551	*1.49*
				1.29	7.00[g]	7.294	*4.20*	6.79	*−2.99*	7.04	*0.57*
				1.2	6.75[a]	6.881	*1.94*	–	–	6.731	*−0.28*
				1.1	6.18[g]	6.398	*3.53*	6.09	*−1.43*	6.39	*3.40*
				0.7	4.65[g]	4.551	*−2.13*	4.62	*−0.64*	5.02	*7.96*
				0.56	4.05[g]	4.026	*−0.59*	4.11	*1.36*	4.55	*12.3*
32	R-SALT (s)	$C_3H_6N_6O_3$	285.85	1.57	7.80[b]	8.18	*4.87*	–	–	7.608	*−2.46*
33	TATB (s)	$C_6H_6N_6O_6$	−154.18	1.88	7.76[g]	7.859	*1.28*	7.70	*−0.76*	7.78	*0.26*
				1.83	7.58[g]	7.707	*1.68*	7.55	*−0.39*	7.63	*0.66*
34	TETRYL (s)	$C_7H_5N_5O_8$	19.50	1.73	7.72[g]	7.725	*0.06*	7.94	*2.83*	7.78	*0.78*
				1.7	7.56[f]	7.634	*0.98*	7.84	*3.65*	7.68	*1.59*

Table 1. continued

No	Name (Phy. State)	Molecular formula	ΔH_f	ρ_0	D_{exp}	D_{ANN}	%Dev	D_{Kesh}	%Dev	D_{KJ}	%Dev
				1.68	7.50[g]	7.571	*0.95*	7.77	*3.57*	7.62	*1.60*
				1.36	6.68[g]	6.49	*−2.84*	6.68	*0.00*	6.63	*−0.75*
				1.2	6.34[g]	5.906	*−6.85*	6.13	*−3.27*	6.13	*−3.31*
35	TNB (s)	$C_6H_3N_3O_6$	−43.51	1.64	7.27[b]	7.175	*−1.31*	–	–	7.152	*−1.62*
36	TNETB (s)	$C_6H_6N_6O_{14}$	−597.56	1.6	7.76[d]	7.726	*−0.44*	–	–	–	–
37	TNT (s)	$C_7H_5N_3O_6$	–66.90	1.64	6.93[c]	6.95	*0.29*	7.20	*3.94*	6.97	*0.58*
				1.6	6.90[c]	6.873	*−0.39*	–	–	–	–
				1.45	6.50[g]	6.603	*1.58*	6.61	*1.62*	6.42	*−1.23*
				1.36	6.20[g]	6.438	*3.84*	6.32	*1.97*	6.16	*−0.65*
				1.14	5.59[a]	5.944	*6.33*	–	–	5.515	*−1.34*
				1.06	5.25[f]	5.715	*8.86*	5.38	*2.45*	5.30	*0.95*
				1.051	5.19[a]	5.688	*9.64*	–	–	5.258	*1.31*
				1.0	5.00[g]	5.524	*10.00*	5.19	*3.80*	5.12	*2.40*
				0.8	4.34[g]	4.783	*10.14*	4.56	*5.09*	4.54	*4.61*
				0.73	4.20[g]	4.499	*7.12*	4.34	*3.36*	4.35	*3.57*

s – solid, l – liquid, Experimental values are taken from [a] – [6], [b] – [7], [c] – [12], [d] – [13], [e] – [14], [f] – [15], [g] – [16], [h] – [17]

predicted values of these explosive compositions. It shows how the computed values compare with similar values predicted by Keshavarz et al. [10] and KJ [6] methods. It is seen that the maximum % deviation of the ANN model is 10.14%. Among the 74 data points, 64 data points have % deviation less than 5% and 10 data points have % deviation from 5–10%.

Also among the 37 explosives used for validation, 25 explosives (constituting to 53 data points) have not been used in training set and 12 explosives (constituting to 21 data points) have been used in training set but at different loading density. This obviously shows that prediction can be done for a wide range of explosives. It can be noted from [6] that the detonation velocity varies with loading density. It is possible to find the variation of detonation velocity with the loading density using the ANN model. Figure 6 shows such variation predicted by the ANN model for two explosives, namely, TNT and RDX. Experimental values were taken from [14–16] at different loading densities.

It can be seen that there is a good match between the predicted and experimental values and the trend predicted is in good agreement with literature. Also, the explosives TNT and RDX are part of the data that were not used in training the ANN model as mentioned above. But the model is able to predict with good accuracy over a range of loading densities. This further corroborate the inner layer refining within the ANN model. The model can thus effectively predict D given the density of the explosive without carrying out any experiment. Since the empirical methods such as Keshavarz method [9] and RP method [7] show the importance or at least emphasize on the use of theoretical maximum density for detonation velocity, we checked to see how the ANN model can predict at the maximum density for the explosives.

Table 2 shows the ANN predicted detonation velocity compared with empirical models (keshavarz [9] and RP method [7]) at the maximum loading densities. In Table 2,

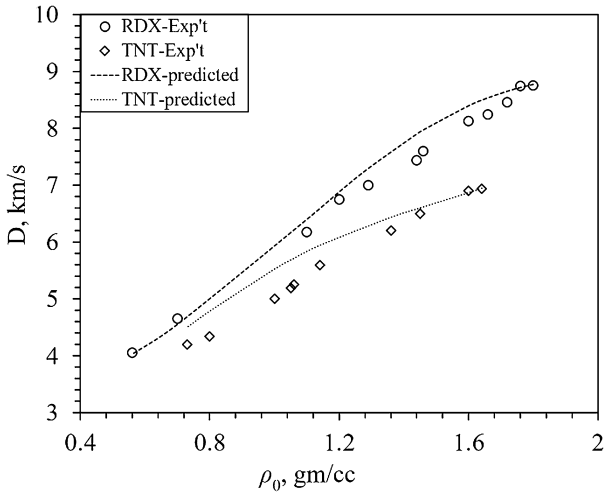

Figure 6. Detonation velocity variation with loading density predicted by ANN model 1 compared with the experimental detonation velocity.

among the 30 explosives shown, 21 explosives were not used in training set and 9 explosives were used in training set but at different loading density. The ANN is able to give good accurate prediction. From Table 1 it can be noted that though the % deviation is less than 5% for most of the data points, while predicting for lower loading densities, the % deviation seems to increase but still is less than 10%. On the other hand if we see Table 2, in all the data points, the ANN model is able to predict detonation velocity with % deviation less than 5%. So it is fair to say that the ANN model is good in predicting over a wide range of loading densities with relatively better accuracy at higher loading densities and maximum loading density. Also from Table 1 and Table 2 it can be seen that the ANN model is good at predicting for different CHNO explosives i.e., pure ex-

plosives (solid and liquid) and mixtures (solid and liquid). Thus the model is a good generalized model for predicting detonation velocity for a wide range of CHNO explosives at different loading densities. Comparing the three methods (Keshavarz method, KJ method and ANN) it can be said that both KJ and Keshavarz method have good predictive capability but Keshvarz method is better than KJ method in predicting detonation velocity for loading densities lesser than 1. The ANN model is on par with the keshavarz method with the added advantage that it is very simple to use and no detailed information about the detonation products are needed to calculate the detonation velocity.

It is not that the ANN model work for all explosives without exceptions. Ammonium nitrate (AN) and AN based explosives like amatol 80/20 (80/20 AN/TNT) appears to show large deviation of over 20% as shown in Figure 7. Ammonium nitrate explosive and explosive mixtures containing ammonium nitrate is said to exhibit non-ideal behavior [11] unlike all the other explosives considered in the dataset. The empirical method of Keshavarz et al. [10] could not treat this behavior of ammonium nitrate and explosive mixtures of ammonium nitrate and they had to come up with an improved empirical model to account for this [11]. This non-ideal behavior of the explosive along with the lack of more data for the ANN model on AN and AN mixtures could be a reason for the ANN to not predict detonation velocity of these explosives accurately (since the accuracy of ANN model depends on the quality and quantity of data available to train). So for direct problem, taking into account all the above discussion, it can be said that the ANN model 1 can predict with good accuracy and versatility, the detonation velocity of wide range of CHNO explosives (pure and mixtures, solid and liquid) at different loading densities with limitation of non-ideal explosives like AN and mixtures of AN.

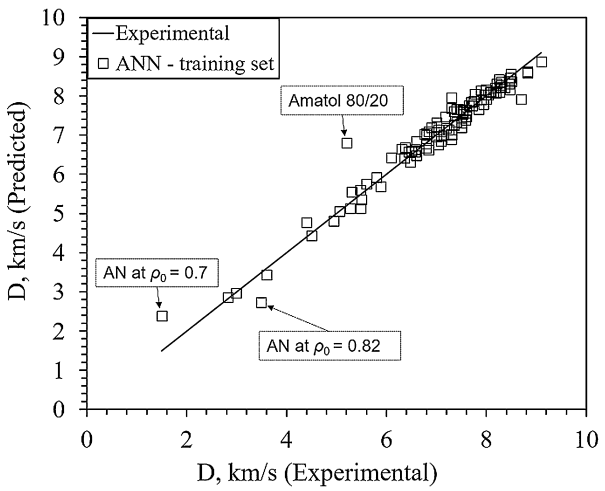

Figure 7. Scatter graph of training set, showing the high % deviation scatter points for ammonium nitrate (AN) and Amatol 80/20.

3.2 Prediction of Elemental Composition: Inverse Problem

Finding new chemical compositions to obtain a predetermined detonation velocity can be a very useful tool for engineers and scientists dealing with explosives. Most of the explosives have energetic groups like nitro, nitrato along with fuel elements like C, H structured in a fashion to make the molecule more energetic. The order of chemical bonds within the molecule, elemental constitution of the bonds, strain built into the structure, associated heat of formation and dissociation, density, crystal structure etc. play combinatorial roles in deciding the final explosive property of a given explosive. An explosive composition can be a concoction or a single molecule. Nitrated explosives and molecules containing catenated nitrogen in different forms have the flexibility of having an engineered chemical composition accomplished through controlled synthetic routes. Nitrogen and oxygen elements can hence be assumed to be within control of the maker of explosive composition.

ANN model 2 developed for the inverse problem can be used to get a prediction of the chemical composition of N and O, given the C and H composition along with detonation velocity, TMD and physical state. Such a reverse prediction using data science methods like ANN, to our knowledge, has not been attempted before for explosives. The data used for training the model is given in Table S2. The compounds selected have diverse structural and molecular features and do not belong to any particular class of explosives. The values for N and O after training shows good agreement with actual values. This trained model was subsequently used for predicting N, O composition of another set of 9 explosives again with varied structural and molecular features. A possible proper prediction of intended characteristics thus eliminates any structural or thermodynamic attributes that relates to the explosive properties. Table 3 shows the comparison between the actual N and O composition of the explosives and ANN predicted N and O composition. It can be seen that the ANN model gives a prediction very close to the actual composition for the selected explosives. This result could perhaps highlight the potential and plausibility of developing ANN models for such reverse mapping.

4 Conclusions

In this paper, we present the possible usage of artificial neural network (ANN) method for prediction of detonation velocity that can be of use in high energetic materials research. ANN ingeniously allows prediction in regimes unexplored in experimental studies. The model 1 was shown to have fairly good prediction capability and versatility in predicting detonation velocity of wide range of CHNO explosives at various loading densities, effect of density on detonation velocity and possible prediction of deto-

Table 2. Comparison of predicted detonation velocity D by ANN and the Keshavarz method [9] and RP method [7] at maximum loading density with experimental data for CHNO explosives; ΔH_f in kJ mol^{-1}; ρ_0 in g cm^{-3}; all D data in km s^{-1} (Direct problem)..

No	Name (Phy. State)	Molecular formula	ΔH_f	ρ_0	D_{exp}	D_{ANN}	%Dev	D_{Kesh}	%Dev	D_{RP}	%Dev
1	ABH (s)	$C_{24}H_6N_{14}O_{24}$	485.34	1.78	7.60[b]	7.775	*2.30*	7.92	*4.26*	7.48	*−1.63*
2	BTF (s)	$C_6N_6O_6$	605	1.90	8.61[b]	8.614	*0.05*	8.85	*2.79*	8.43	*−2.14*
3	Cyclotol 50/50 (s)	$C_{2.22}H_{2.45}N_{2.01}O_{2.67}$	0.04	1.63	7.66[g]	7.781	*1.58*	8.07	*5.30*	7.81	*1.99*
4	Cyclotol 60/40 (s)	$C_{2.04}H_{2.5}N_{2.15}O_{2.68}$	4.81	1.74	8.09[g]	8.195	*1.30*	8.13	*0.45*	8.07	*−0.24*
5	Cyclotol 65/35 (s)	$C_{1.96}H_{2.53}N_{2.22}O_{2.68}$	8.33	1.72	8.04[g]	8.184	*1.79*	8.15	*1.43*	8.18	*1.78*
6	Cyclotol 70/30 (s)	$C_{1.87}H_{2.56}N_{2.29}O_{2.68}$	11.13	1.73	8.06[g]	8.251	*2.37*	8.19	*1.55*	8.31	*3.12*
7	Cyclotol 77/23 (s)	$C_{1.75}H_{2.59}N_{2.38}O_{2.69}$	14.98	1.743	8.25[g]	8.33	*0.97*	8.23	*−0.29*	8.48	*2.83*
8	DATB (s)	$C_6H_5N_5O_6$	−98.70	1.84	7.67[b]	7.786	*1.51*	7.52	*–1.91*	7.70	*0.33*
9	DIPAM (s)	$C_{12}H_6N_8O_{12}$	−28.45	1.79	7.50[b]	7.753	*3.37*	7.64	*1.91*	7.57	*0.94*
10	EDC-11 (s)	$C_{1.99}H_{2.78}N_{2.23}O_{2.63}$	4.52	1.782	8.21[f]	8.344	*1.63*	8.14	*−0.83*	8.02	*−2.39*
11	EDC-24 (s)	$C_{1.64}H_{3.29}N_{2.57}O_{2.57}$	18.28	1.776	8.71[f]	8.5	*−2.41*	8.26	*−5.18*	8.30	*−4.70*
12	EDNA (s)	$C_2H_6N_4O_4$	−103.81	1.71	8.23[b]	8.426	*2.33*	7.78	*−5.47*	8.31	*0.96*
13	EGDN (l)	$C_2H_4N_2O_6$	−242.84	1.48	7.30[b]	7.25	*−0.68*	7.51	*2.85*	7.49	*2.62*
14	EXP D (s)	$C_6H_6N_4O_7$	−386.39	1.72	7.36[b]	7.257	*−1.4*	7.35	*−0.19*	7.40	*0.57*
15	HNS (s)	$C_{14}H_6N_6O_{12}$	78.20	1.74	7.13[b]	7.065	*−0.91*	6.86	*−3.74*	6.83	*−4.16*
16	NG (l)	$C_3H_5N_3O_9$	−371	1.6	7.70[b]	7.575	*−1.62*	7.77	*0.88*	7.44	*−3.42*
17	NM (l)	CH_3NO_2	−113	1.13	6.35[g]	6.295	*−0.87*	6.44	*1.35*	5.51	*−13.24*
18	NONA (s)	$C_{18}H_5N_9O_{18}$	114.64	1.78	7.56[f]	7.97	*5.42*	7.35	*−2.80*	7.31	*−3.26*
19	NQ (s)	$CH_4N_4O_2$	−92.5	1.78	8.59[g]	8.349	*−2.8*	8.64	*0.55*	8.27	*−3.69*
20	ONT (s)	$C_{18}H_6N_8O_{16}$	82.72	1.80	7.33[f]	7.589	*3.53*	6.96	*−5.09*	6.97	*−4.94*
21	PBXC-116 (s)	$C_{1.97}H_{3.75}N_{2.36}O_{2.47}$	4.52	1.65	7.96[f]	8.14	*2.26*	8.14	*2.32*	7.54	*–5.22*
22	PBXC-119 (s)	$C_{1.82}H_{4.11}N_{2.21}O_{2.69}$	18.28	1.635	8.08[f]	8.273	*2.39*	8.14	*0.87*	7.67	*−5.08*
23	Pentolite 50/50 (s)	$C_{2.33}H_{2.37}N_{1.29}O_{3.22}$	−100	1.65	7.47[f]	7.424	*−0.61*	7.13	*−4.51*	7.67	*2.78*
24	Picric acid (s)	$C_6H_3N_3O_7$	−214.60	1.76	7.57[b]	7.477	*−1.23*	7.18	*−5.15*	7.36	*−2.73*
25	RDX (s)	$C_3H_6N_6O_6$	61.55	1.83	8.85[b]	8.811	*−0.44*	9.01	*1.85*	8.95	*1.08*
26	R-SALT (s)	$C_3H_6N_6O_3$	285.85	1.57	7.80[b]	8.18	*4.87*	8.00	*2.60*	7.89	*1.17*
27	TATB (s)	$C_6H_6N_6O_6$	−154.18	1.95	7.94[b]	8.055	*1.45*	7.73	*−2.63*	7.87	*−0.85*
28	TETRYL (s)	$C_7H_5N_5O_8$	19.50	1.73	7.91[b]	7.725	*−2.34*	7.50	*−5.13*	7.78	*−1.62*
29	TNB (s)	$C_6H_3N_3O_6$	−43.51	1.64	7.27[b]	7.175	*−1.31*	7.11	*−2.22*	7.27	*0.04*
30	TNT (s)	$C_7H_5N_3O_6$	−66.90	1.64	6.95[b]	6.95	*0.00*	6.91	*−0.64*	6.67	*−4.04*

s – solid, l – liquid, Experimental values are taken from [b] – [7], [f] – [15], [g] – [16].

Table 3. Chemical composition predicted by ANN model 2 vs actual chemical composition (Inverse problem).

	Actual composition		Composition predicted by ANN	
	N	O	N	O
BTF	6	6	7	4
EGDN	2	6	2	6
EXP D	4	7	4	7
MN	1	3	2	3
NM	1	2	2	3
NIBTN	4	11	4	11
RDX	6	6	6	7
TNB	3	6	4	5
TNT	3	6	4	6

nation velocity in unexplored regime. Model 2 was able to predict N and O composition of C, H, N and O based explosive molecule for a targeted detonation velocity. This facilitates possible control on nitration or introduction of other N, O based explosive groups in a molecule. Such predictive capabilities are a great tool for engineers and scientists working with high energy materials to assess and reevaluate compositions for a set of targeted properties.

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