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Burning Rate Prediction of Solid Rocket Propellant (SRP) with High-Energy Materials Genome (HEMG)

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Abstract: High-energy materials genome (HEMG) is an analytical and calculation tool that contains relationships between variables of the object, which allows researchers to calculate the values of one part of the variables through others, solve direct and inverse tasks, predict the characteristics of non-experimental objects, predict parameters to obtain an object with desired characteristics and execute virtual experiments for conditions which cannot be organized or have difficultly being organized. HEMG is based on experimental data on the burning rate of various high-energy materials (HEMs) under various conditions, on the metadata on the quantum and physicochemical characteristics of HEMs components as well as on thermodynamic characteristics of HEMs as a whole. The history and current status of the emergence of HEMG are presented herein. The fundamental basis of the artificial neural networks (ANN) as a methodological HEMG base, as well as some examples of HEMG conception used to create multifactor computational models (MCM) of solid rocket propellants (SRP) combustion, is presented.

Keywords: high-energy materials genome; artificial neural networks; burning rate; multifactor computational models

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1. Introduction

When researching into the area of high-energy materials (HEMs), the goal is always to search for new HEMs with improved properties. There is currently no standard practice for researchers and developers to disclose predictive algorithms and in silico methods for developing new propellants with desirable characteristics. Therefore, generally, it was necessary to conduct many expensive and hazardous experiments to obtain a burning rate or to determine the optimal HEMs compositions. There exist a large number of experimental data about the combustion characteristics of HEMs [1–3], while there are several disadvantages for HEM investigation, such as expensive cost, safety risks, etc. With the rapid development of computer simulation science and combustion diagnosis technology, the performance prediction of solid rocket propellant (SRP) has gained much attention from researchers worldwide. The prediction of burning rate of SRPs is an important aspect of analysis, which has important theoretical significance to reveal the combustion mechanism of SRP. For example, Zhang Xiaoping et al. used genetic neural network to simulate the combustion performance of nitrate ester plasticized polyether (NEPE) propellant under high-pressure conditions and proposed 13 characterization parameters. This method has high calculation accuracy, but the model is a purely physical model that does not consider the influence of chemical composition and the structure of propellants [4]. The effect of various factors on the combustion characteristics of SRP can be predicted by using multi-factor calculation model (MCM) non-linear combustion models that are based on artificial intelligence (AI) methods.

In this work, the high-energy materials genome (HEMG) method was introduced. Based on the usage of AI, this solves the problems of creation of MCM of combustion

and detonation. Its history and current status, as well as examples of the results of its application, were presented. In particular, we detailed the use of artificial neural networks (ANN) to create the MCM of combustion of SRP. Additionally, the burning rate of SRP with micro-sized aluminium (mAl) or nano-sized metal (nAl and nNi) particles was calculated by means of ANN, predicted in some cases and then compared to the experimental data.

2. History and Current Status of HEMG

HEMG is based on the experimental data on the combustion and detonation characteristics of various HEMs under various conditions, being based also on the metadata on the quantum and physicochemical characteristics of HEMs components as well as the thermodynamic characteristics of HEM as a whole.

HEMG involves the principles of the Materials Genome Initiative (MGI) for Global Competitiveness that was announced through a whitepaper by the National Science and Technology Council of the USA in June 2011 [5], which is one of starting points of HEMG history.

In 2014, the US National Institute of Standards and Technology presented a strategic plan for the implementation of MGI. In the field of energetic materials (EMs), as a continuation of the MGI idea, the Energetic Materials Genome Initiative (EMGI) was launched as an idea in 2017 and it was marked that if the MGI modes were used in the development of EMs, the efficiency of EMs manufacturing would be greatly enhanced, which will benefit the society [6]. It could be noted that the research corresponding to the idea of MGI at Chuvash State University saw their proposals implemented, and the MCM for combustion and detonation obtained by means of ANN were presented [7,8]. Moreover, the MCM of various SRP combustions were obtained [9], and improved MCM for various SRP combustions and detonations were obtained [10–14].

Nowadays, in the fields of HEMs, the following works dealing with the conception of MGI are worth analysis. For instance, Wang et al. [15] depict how the MGI approach can be used to accelerate the discovery of new insensitive high-energy explosives by the identification of "genetic" features. Kang et al. [16] depict how machine learning (ML), materials informatics (MI), and thermochemical data are combined to screen potential candidates of EMs. To directly characterize the energetic performance, the heat of explosion is used as the target property. The critical descriptors of cohesive energy, averaged over all constituent elements and the oxygen balance, are found by forward stepwise selection from a large number of possible descriptors. With them and a theoretically labeled heat of explosion training data set, a satisfactory surrogate ML model is trained. The ML model is applied to the large databases NIST ICSD (NIST Inorganic Crystal Structure Database, NIST Standard Reference Database Number 3, National Institute of Standards and Technology, Gaithersburg MD, 20899, DOI: https://doi.org/10.18434/M32147, (retrieved on 28 January 2023) and PubChem to predict the heat of explosion. At the gross-level filtering by the ML model, 2732 molecular candidates based on carbon, hydrogen, nitrogen, and oxygen (CHNO) with high heat of explosion are predicted. Afterward, a fine-level thermochemical screening is carried out on the 2732 materials, resulting in 262 candidates with TNT equivalent power index Pe (TNT) greater than 1.5. Raising Pe (TNT) further to larger than 1.8 sees 29 potential candidates be found from the 2732 molecular candidates, all of which are new to the current reservoir of well-known EMs. Yuan et al. [17] remarked that the approach of taming energetic compounds via the permutation of chemical building blocks has gradually reached a crossroads. The future will leverage new tools such as AI to construct the HEMG method. Yang et al. [18] remarked that researchers have begun to apply deep learning methods to the prediction of explosive detonation performance. The deep learning method has the advantage of simple and rapid prediction of explosive detonation properties. However, some problems remain in the study of detonation properties based on deep learning. For example, there are few studies on the prediction of mixed explosives, on the prediction of the parameters of the equation for the state of explosives, or on the application of explosive properties to predict the formulation of explosives. Based on an ANN model

and a one-dimensional convolutional neural network model, three improved deep learning models were established. Tian et al. [19] marked that the prediction of the properties of EMs using ML has been receiving more attention in recent years. This review summarized recent advances in predicting energetic compounds' density, detonation velocity, enthalpy of formation, sensitivity, the heat of the explosion, and decomposition temperature using ML. Moreover, it presented general steps for applying ML to the prediction of practical chemical properties from the aspects of data, molecular representation, algorithms, and general accuracy. Additionally, it raised some controversies specific to ML in EMs and its possible development directions. Important information related to MGI can be found at [20]. In June 2022, the MGI Fifth Principal Investigator Meeting took place. It was noted that techniques on well-known species of CHNO-based EMs, such as HMX, PETN, TNT, RDX, TATB and CL-20, were developed [21]. This promises rich scientific advances in the data-driven design of next-generation EMs.

In conclusion, it can be noted that the works using the MGI conception have begun to appear for EMs in recent years [9–19,21]. Much attention has been paid to the development of new molecules of insensitive high-energy explosives and the implementation of screening of potential candidates of advanced EMs from the point of view of the heat of explosion. Multifactor computational models are being created that allow researchers to solve the direct task—prediction of explosive detonation properties, in particular to approximate the dependence of the detonation velocity of explosives on various parameters, predicting energetic compounds' properties. For example, the inverse task of determining the atomic composition of the explosive molecule was solved [18,22,23]. The methodology and know-how for creating MCM of HEMs combustion by means of ANN, as well as examples of the results of the application of ANN for creating the MCM of combustion of various propellants, was outlined in [24].

3. Methodology

The application of ANN, one of the best tools for creating MCM of experimental data, is based on the Kolmogorov–Arnold theorem [25–27] and its special cases considered by Hecht-Nielsen [28]. From a computational point of view, ANN is a structure that includes a certain number of processing elements and which executes a fixed set of mathematical functions. This processing element is called an artificial neuron (AN). It consists of an input vector (Xi), synapses, a summator, a nonlinear transfer function, and an output signal value, as shown in Figure 1 [8].

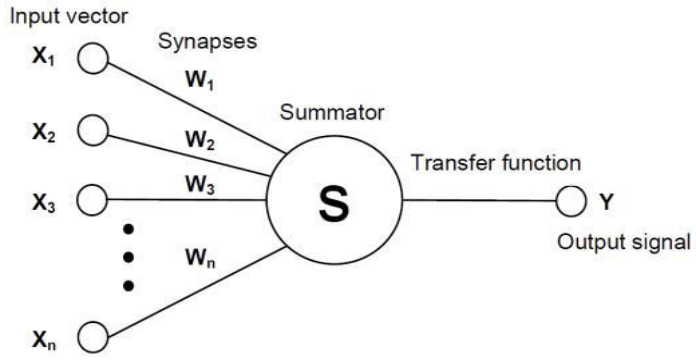


Figure 1. A scheme of an elementary processor of an artificial neuron.

The executive equation of a neuron is determined according to the following operations:

$$S = \sum_{i=1}^{n} X_i W_i \quad (1)$$

$$f(S) = \frac{1}{1 + e^{-\alpha S}} \quad (2)$$

$$Y = f(S) \tag{3}$$

The task of synapses is to multiply the input vector components, X_i, by a number characterizing the synapse strength (it is called synaptic weight, or W_i). These values obtained are summed and the sum is fed into the transfer function, Y, whose role is played by a monotonous function of one argument (usually sigmoid function $f(S)$). Thus, AN maps the vector X_i to a scalar value Y.

The simplest kind of ANN is feed-forward ANN, whose neurons are grouped into layers. The structure of feed-forward ANN is shown in Figure 2 [8].

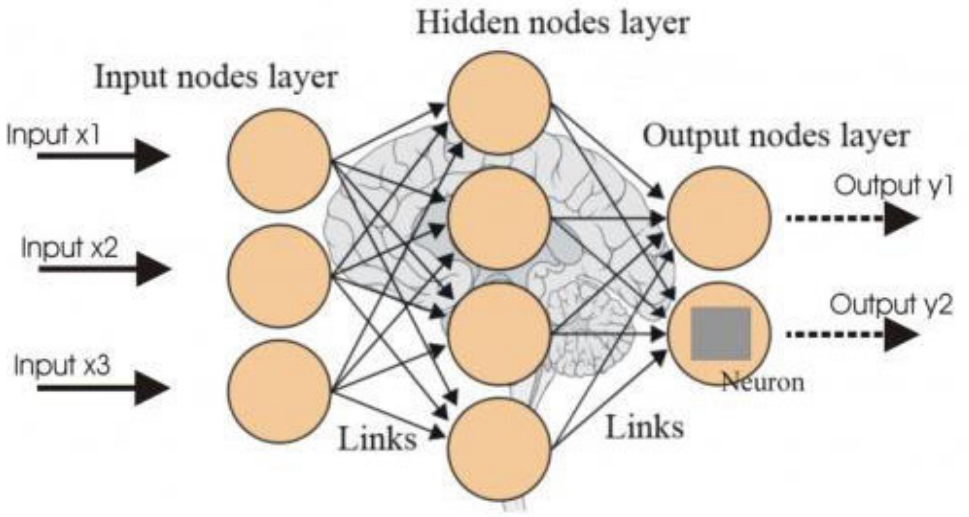


Figure 2. The structure of feed-forward ANN.

As seen in Figure 2, its structure consists of one input nodes layer (3 input nodes), one hidden layer (4 neurons) and one output layer (2 neurons), with each layer relating to its neighboring layer in "all-to-all" manner. Input nodes serve only as signal sources, while the other neurons perform the computations described above.

This computational structure can approximate the dependencies between the input variables and target (output) variables (functions) of an object after its training on a set of experimental data. The essence of training is to select the correct synaptic weights. In the process of training, weights of all synapses are determined from the requirement that ANN should map all known input vectors to the known corresponding values of the target variables with minimum errors.

This process is organized as follows. The initial synaptic weights are set using a random number generator. Then, a random input vector of real data is selected and fed into the ANN. The ANN calculates an output value, it is compared with the expected output value and the respective error is calculated. Using the "error back propagation" algorithm based on the classic gradient descent method [29–31], synaptic weights are changed by certain values. After that, a new input vector of real data is randomly selected and the whole weight update procedure is repeated. The procedure is repeated until an acceptable difference between the values computed by ANN and real values of the target variable is reached. The number of training cycles can be more than 500–1000.

The resulting ANN is able to map any input vector which is close to the vectors used during training into the respective value of the target variable i.e., it can approximate the dependence of a target variable on input factors.

The organization of real data to be used for ANN training is very important. The data for ANN training (consisting of input variable value vectors and output values corresponding to them) can be formed by means of various techniques. They can contain data measured in real experiments or data obtained from numerical simulations; they can contain data of both types when these data can complement each other. The data must be

cleared, that is, contradictions, duplicates, anomalous values must be excluded. The data should be evenly distributed over the area of the input vector space, and it is necessary to avoid large differences in data density in different parts of this area (this is the requirement for data to be equally weighted).

The data should be supplemented with metadata containing additional information about the object, for example, physical or chemical constants characterizing the object under study, the parameters of the technology for creating the object, etc. The use of metadata as additional data not only increases the accuracy of the ANN model, but it also allows a deeper understanding of the physicochemical nature of the objects of research and the fine details of the mechanism of the processes under study.

Another significant circumstance is proper choice of ANN structure for which certain theoretical and empirical rules exist. For example, one of general rules (confirmed by our experience) is that the number of synapses should be 3–5 times less than the number of input vectors (examples) used in training. Use of ANN with a greater number of synapses may lead to the so-called overfitting.

The loss of the ability to generalize means that the ANN remembers training examples well and accurately reproduces the target variables for the training input vectors, but gives erroneous values of the target variables for the input vectors that it does not use in training.

To find out if the ANN has the ability to generalize the dependencies contained in the data, the following approach is used. In the process of training, the input vectors (a set of examples) are divided into two groups. A large group is used for training, and a smaller group is used only to check the ANN prediction accuracy. If the ANN accuracy in both groups is approximately the same, the ANN is not retrained and has the ability to identify and generalize the dependencies of existing data.

One more rule that has been empirically established is that it is better to use two separate ANN for each of the two "outputs" than one ANN for both "outputs" (Figure 2). The general principle for ANN structure selection is as follows. For the majority of tasks, two hidden ANN layers are sufficient to obtain an acceptable error level. Therefore, using ANN with more than two hidden layers can hardly make sense in many cases. Moreover, accuracy of networks with a single hidden layer (Figure 2) is often quite good for problems of physics and natural science where dependencies are deterministic. The final choice of the optimal ANN structure for each research task is carried out empirically by checking the exactness of different ANN (for example, with a different number of AN in the hidden layer).

It should be noted here that all questions of the methodology of ANN use for approximating experimental data have been well worked out at present, both from a theoretical and practical point of view. There exist a number of academic (free) and professional software packages which support all steps of data pre-processing, ANN training, model results visualization, model quality evaluation and validation. These make modeling experimental data simple and convenient.

Therefore, at present, it is possible to put forward the motto that experimental work cannot be considered complete until an MCM of experimental data has been created.

We believe that an autonomous executable module of the ANN model created by the authors of the article should be a mandatory supplement to any scientific article. This is explained as follows. A correctly created ANN model is, first, the most complete form of presentation of experimental results, since the ANN model contains the relationships between all the variables of the experiment. This will allow any reader of the article, having received the autonomous executable module, to independently examine in detail all the regularities contained in the ANN model and visualize in the form of graphs those regularities that the authors of the article could not cite in the article due to limitations on the volume of the article.

An additional advantage of the autonomous executable module of the ANN model is that, with its help, the reader of the article can conduct "virtual experiments", setting such

combinations of factor values that were not investigated in the published article. Examples of possible scenarios for virtual experiments and the results obtained are presented in [24].

The results of the virtual introduction of copper isobutyrate catalyst into various mixtures of copper phthalate + lead catalyzed by soot greatly changes both the value of the burning rate and the dependence of the burning rate on pressure [32].

The results of of virtual simultaneously embedding two or more different types of metal powder Al, Ti, Ni, and Zr into propellants with varying composition are depicted in [12]. The results depict that the value of the burning rate and the graph of the dependence of the burning rate on the pressure vary in a complex way depending on the type of metal and the amount of simultaneously embedded metals. The results of the virtual simultaneous embedding of two additives differing in size (micro-size and nano-size) in the propellants composition are depicted in [33]. The results of virtual simultaneous use of mAl/PbO (micro-size) and nAl/PbO (nano-size) indicate that the value of the burning rate and the graph of the dependence of the burning rate on pressure change significantly.

Virtual experiments can also be carried out to execute unique experiments for such combinations of factor values that cannot be organized or are difficult to organize. The results of virtual use of only monodisperse AP particles in the propellant compositions are depicted in [34]. The two real propellant compositions have polydisperse AP particles with average sizes of AP particles 45.8 $\pm$ 30 μm and 399.6 $\pm$ 82 μm. The results of virtual use of only monodisperse AP particles 45.8 μm and 399.6 μm show that the monodispersity of AP particles does not strongly affect the combustion rate or the form of dependence of the combustion rate on pressure for both cases.

In addition to the above, one more very interesting case should be noted when the use of ANN is justified. Our experience shows that the root-mean-square (RMS) error of the ANN model is always less than the RMS error of the experimental data used to create the ANN model. This allows the ANN model to be used as a means of checking the quality of the experiment as a whole! Moreover, it can do so both from the point of view of the measurement error of the variables of the experiment, and from the point of view of the correctness of the experiment, that is, from the completeness of taking into account all the factors affecting the goal of the experiment.

In cases where the RMS error of the ANN model is too large (for example, when the RMS error of the ANN model is more than 10^{-3}), it is necessary to improve the accuracy of the experimental variables measurement and (or) change the formulation of the experimental problem, trying to take into account additional factors affecting the goal function of the experiment.

An example of the use of additional factors (metadata) that affect the goal function of the experiment, i.e., the detonation velocity, is presented in [22,23]. In contrast to [11], in which only the numbers of C, H, N, O atoms in the explosive molecules were used as input data, in [22,23] not only were the numbers of C, H, N, O atoms in the explosive molecules used, but so were combinations of the ratio of the number of atoms C, H, N, O to each other (C/H, N/O). These combinations can be considered as metadata that reflect a structure of the ratio of the explosive molecules. The evaluation of the quality of the model indicated that the RMS error is 0.00025. The maximum relative error is less than 1% over the entire range of detonation velocities, except for very low (about 1.5 km/s) and very high (more than nine km/s) detonation velocities. These errors are several times smaller than errors for the model presented in [11]. The reduction in errors and the improvement in the quality of the model occurred precisely due to the input of metadata, reflecting the structure of chemical bonds in the explosive molecule as factors into the model.

4. Results and Discussion

4.1. Experiment

The base set of burning rate data was taken from [35]. The set consists of data about combustion of RDX-CMDB and CL-20-CMDB propellants with different nanopowders and contents:

- 73.5% NG/NC + 19.5% burning rate inhibitor + 4.0% catalyst + 3.0% additives with and without nAl;
- 63.0% NG/NC + 2.3% catalyst + 2.8% additives + 26% RDX + 4.6% diethyl phthalate (DEP) + 2.6% (nAl + Al_2O_3) with and without nAlN;
- 63.4% NG/NC + 5.85% catalyst + 4.75% additives + 24% HMX with and without nDPN;
- CL-20-CMDB propellants formulation with different mass fraction of nNi;
- RDX-CMDB propellants with different mass fractions of nNi.

The base set is prepared in a special type [36] of that modeling by means of ANN demands.

4.2. Modelling

All models were obtained by using ANN that included in analytical platform Deductor (https://basegroup.ru/deductor/description (accessed on 28 January 2023).

4.2.1. Direct Task

The direct task reveals dependences of the burning rate (goal function of models) on the various factors. In our case, ANN structure (Figure 3) for solving the direct task consists of one input layer (17 neurons which correspond to 17 factors), one hidden (inner) layer (5 neurons) and one output layer (1 neuron which corresponds to goal function).

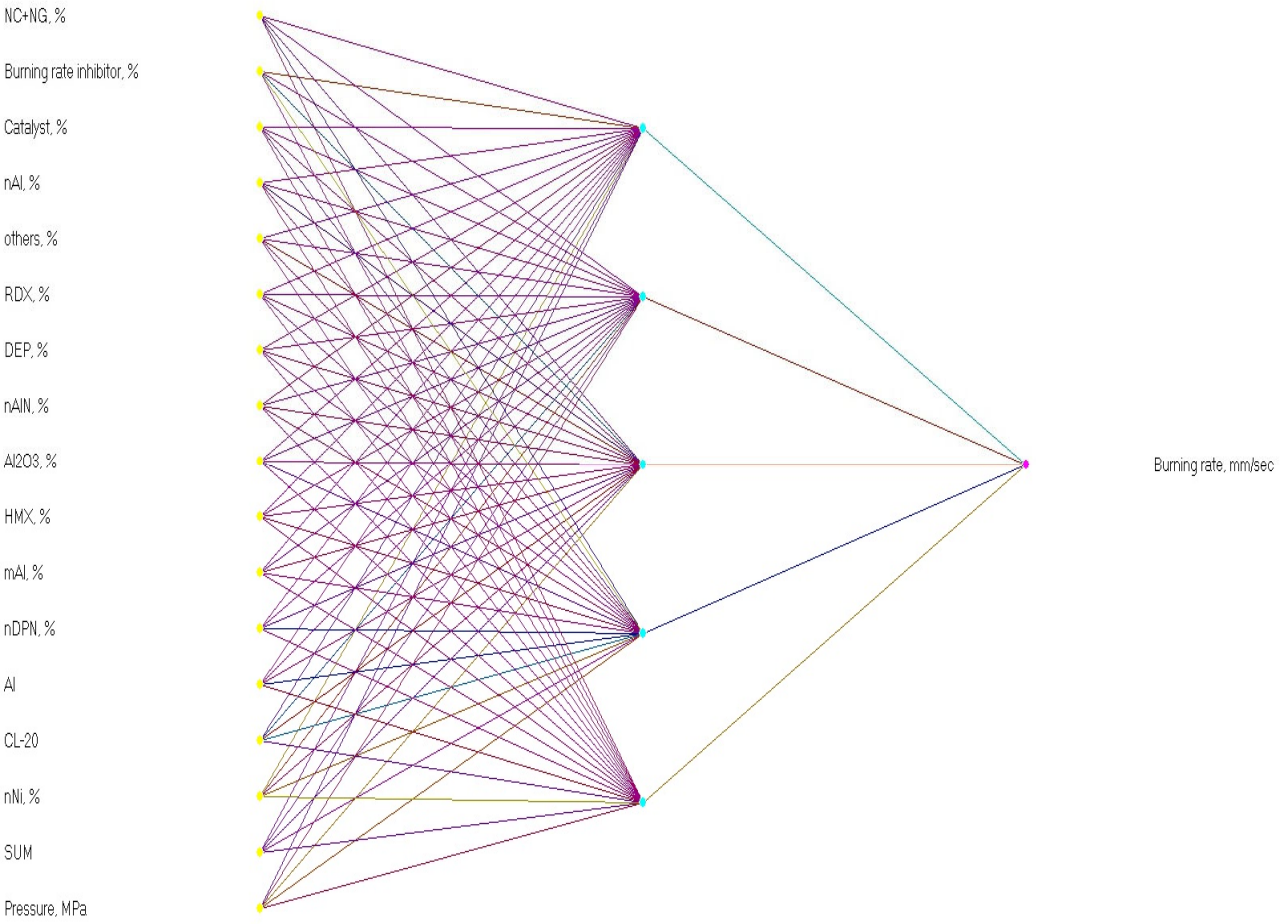


Figure 3. ANN structure for solving the direct task.

This calculation structure, after training on the experimental data, allows the determination (calculation) of the burning rate value for any set of factors values.

The advantage of the analytical platform Deductor is the automatic execution of quality assessments of the ANN model obtained. A portion (95%) of the full data set was randomly selected and used for training, and the remaining data (5%) was used for model testing (validation) only. Both the testing and training procedures are run simultaneously. The quality assessments of the ANN model obtained depicts that root-mean-square error of the ANN model training procedure equals 3.4×10^{-4} for 78% of the training data set and that the root-mean-square error of the ANN model testing equals 5.1×10^{-4} for 71% of testing data set.

It is important to note that the root-mean-square error of the testing procedure on the data that have not been used for training is about equal to the root-mean-square error of the training procedure. This observation confirms that the overfitting of ANN structure is not present.

The examples of the results of calculation of the ANN MCM that solves a direct task (two cases for various set of factors) and if two graphs of the dependence of burning rate on pressure are depicted in Table 1 and in Figures 4 and 5. In Table 1, the dependence of the burning rate on pressure value and the quantity of additives, denoted with the names "others" and nNi, it depicted.

Table 1. Examples of results of calculation of the ANN MCM that solves the direct task.

Input Factors	Values in Case 1	Values in Case 2
NC + NG, %	82.5	82.5
Burning rate inhibitor, %	0	0
Catalyst, %	5.75	5.75
nAl, %	0	0
Others, %	6.25	5.75
RDX, %	0	0
DEP, %	0	0
nAlN, %	0	0
Al_2O_3, %	0	0
HMX, %	0	0
mAl, %	0	0
nDPN, %	0	0
Al	5.5	5.5
CL-20	0	0
nNi, %	0	0.5
SUM	100	100
Pressure, MPa	15	10
Output Burning rate, mm/s	31.9	34.4

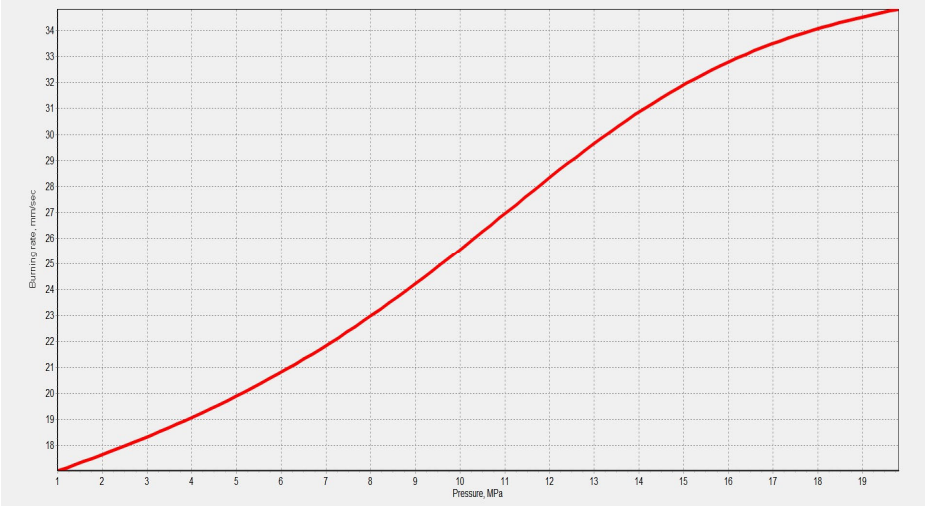


Figure 4. A representative dependence of burning rate on pressure for the case 1 in Table 1.

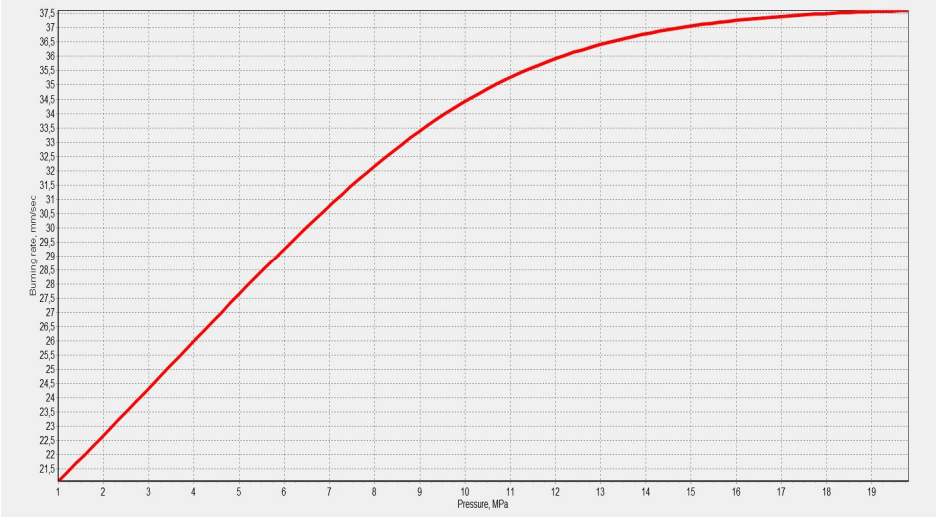


Figure 5. A representative dependence of burning rate on pressure for the case 2 in Table 1.

The graphs like Figures 4 and 5 are obtained, by means of the Deductor, in auto mode in every time the researcher calculates a burning rate and for any set of input values.

The ANN MCM obtained can be considered as a specialized calculator that solves the direct task and contains all the links between the goal and function of the model—the burning rate and 17 factors. It can instantly give the value of the burning rate for any set of factor values and present graphs of the burning rate versus any factor, not just pressure. Much more examples of such results are presented in [24].

4.2.2. Inverse Problem (Task)

The one of possible ANN structure for solving the inverse task (Figure 6) consists of one input layer (17 neurons which correspond 16 factors and 1 goal function—burning rate which we have to obtain), one hidden (inner) layer (5 neurons) and one output layer (1 neuron which corresponds 1 factor—pressure which have to help us to rich the required value of burning rate).

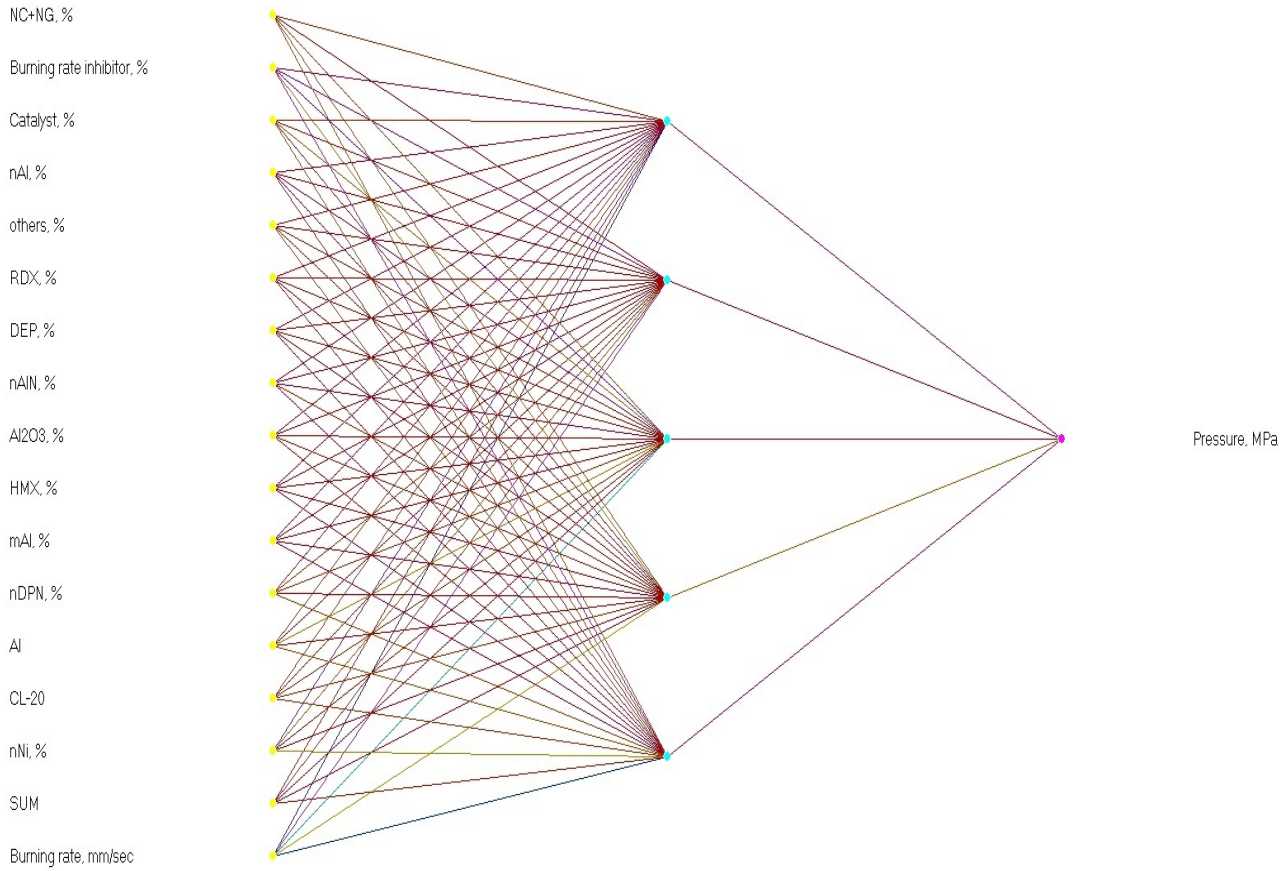


Figure 6. ANN structure for the simplest form of inverse task.

This calculation structure, after training, allows the determination (calculation) of the pressure values that can help us to enrich the required value of burning rate for any set of factors values.

The quality assessments of the ANN model obtained depicts that the root-mean-square error of the ANN model training procedure equals 1.7×10^{-2} for 86% of training data set and that the root-mean-square error of the ANN model testing equals 7.3×10^{-3} for 43% and 1.4×10^{-2} for 29% of testing data set.

The root-mean-square error of the model for solving the inverse task is greater than of the model for solving the direct task. This is quite understandable. The latter is explained by the fact that inverse tasks solved based on experimental data are incorrectly (ill-posed) set, according to Hadamard, from the point of view of pure mathematics. If the requirements for the existence of a solution and the stability of the solution to errors in the input data are satisfied in the case of using an ANN well, then the requirement for the uniqueness of the solution cannot be fully met. First of all, this is due to the significant multifactor nature of the task of determining the pressure that provides one or another burning rate, both since the same burning rate can be obtained both due to a change in pressure (with a constant propellant composition) and due to the composition of the propellant (at a constant pressure).

The examples of the results of that calculation of the ANN MCM that solves the inverse task and the graph of connection of the burning rate and pressure are depicted in Table 2 and Figure 7.

Table 2. The example of result of calculation of the ANN MCM that solves the inverse task.

Input Factors	Values
NC + NG, %	63
Burning rate inhibitor, %	0
Catalyst, %	2.3
nAl, %	0
Others, %	2.8
RDX, %	26
DEP, %	4.6
nAlN, %	1.3
Al_2O_3, %	0
HMX, %	0
mAl, %	0
nDPN, %	0
Al	0
CL-20	0
nNi, %	0
SUM	100
Burning rate, mm/s	18
OutputPressure, MPa	15.2

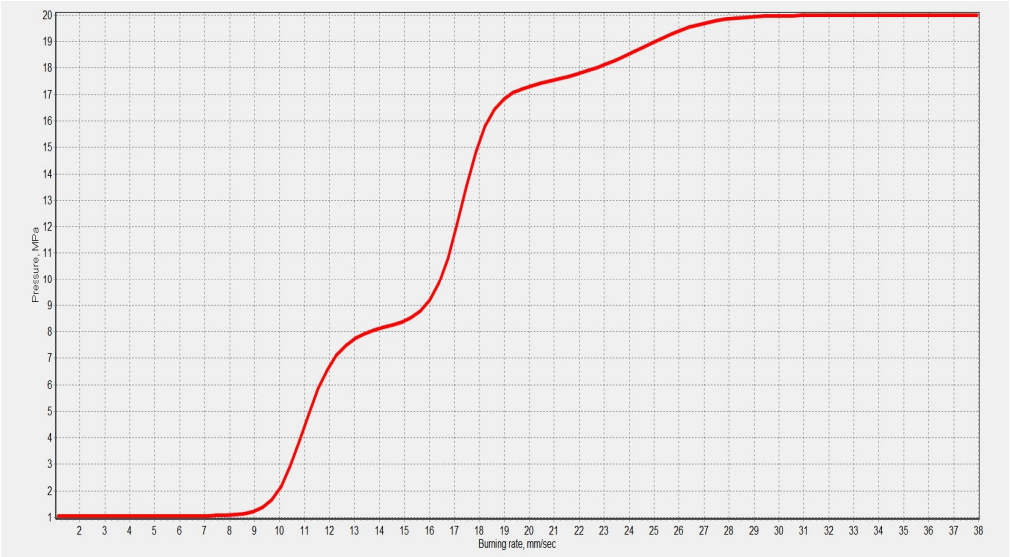


Figure 7. An example of a graph of connection of burning rate and pressure. The graph is valid only for the set of input factors values indicated in Table 2. For other sets of values, the graphs will be different.

The ANN MCM (calculator) that solves the inverse task allows us to solve various problems related to determining the composition of HEM and the level of pressure to needed obtain the required burning rate. We have presented some such results at [24,37].

4.2.3. Virtual Experiments

The ANN MCM for solving a direct task has a very interesting feature. This allows for a virtual experiment. The essence of the virtual experiment was as follows.

The virtual experiments are computational experiments carried out using ANN MCM, and during this such combinations of factor values are established that were not investigated in a real experiment. For example, a virtual experiment includes the extrapolation of the dependencies identified by the ANN model, for example, the task of predicting the values of the burning rate for pressure values for which experiments have not been carried out. Another example of a virtual experiment is a computational experiment, during which such a combination of factor values (such a set of factor values) is specified, for which the real experiment was not carried out.

The result of the virtual experiment is depicted in Table 3 and Figures 8 and 9. In Table 3, on the left is the example of the results of calculation of ANN MCM for solving the direct task for a propellant composition for which real experiments were carried out. On the right is the example of the results of calculation of ANN MCM for solving the direct task for a virtually changed propellant composition.

Table 3. The example of result of calculation of the ANN MCM that executes virtual experiments (right side).

Input Factors	Values for the Real Experiment	Values for the Virtual Experiment
NC + NG, %	63.4	63.4
Burning rate inhibitor, %	0	0
Catalyst, %	5.85	5.85
nAl, %	0	0
others, %	4.75	4.75
RDX, %	0	0
DEP, %	0	0
nAlN, %	0	0
Al_2O_3, %	0	0
HMX, %	24	24
mAl, %	2	2
nDPN, %	0	0.7
Al	0	5.5
CL-20	0	0
nNi, %	0	0
SUM	100	106.2
Pressure, MPa	15	15
Output Burning rate, mm/s	22.3	25.5

During the virtual experiment, we have included such components as nDPN and Al in the propellant composition simultaneously (this composition was not really studied in the experiment). The model instantly calculated the value of the burning rate for the new propellant composition.

4.2.4. Comparison of Predicted Burning Rate with Experimental Data of SRP

The results of experimental research of combustion performance of double-base SRP with micro- and nano-sized additives were taken, dealing with the effects of different nano-sized additives on the burning rate of double-based SRP with such micro- and nano-sized metals. It has been used for the creation of combustion multifactor computational models that solve direct and inverse tasks, and the predicted burning rate of SRP was determined as well. Figure 10 shows the comparison curves of predicted burning rate with the experimental data of SRP. It can be seen that the predicted burning rate data agree

well with the experiments ones. The predicted burning rate curves are smoother than the experiment curves.

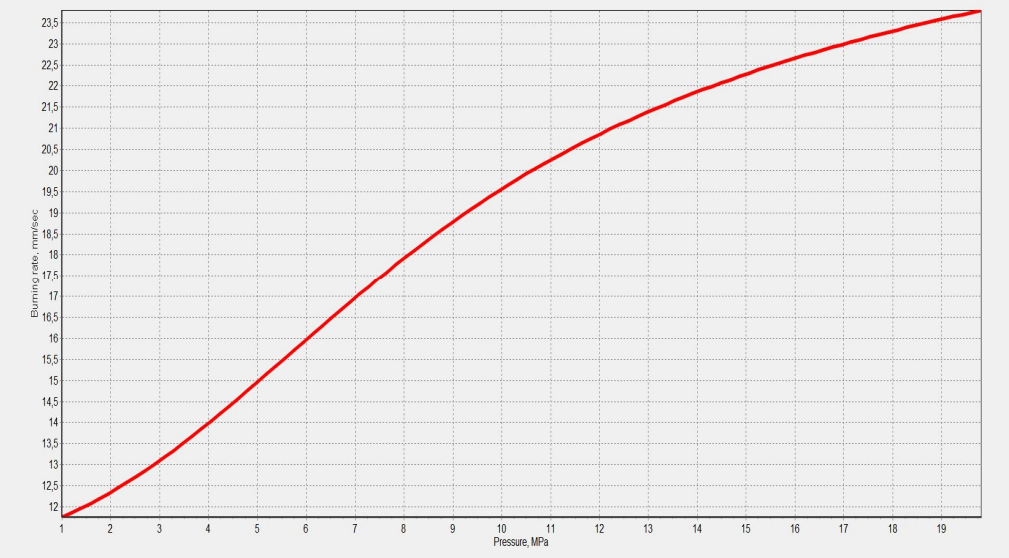


Figure 8. The graphs of the dependence of the burning rate on pressure, corresponding to the results of calculation of ANN MCM for real experiment (left side of the Table 3, direct task for the propellant for which real experiments were carried out).

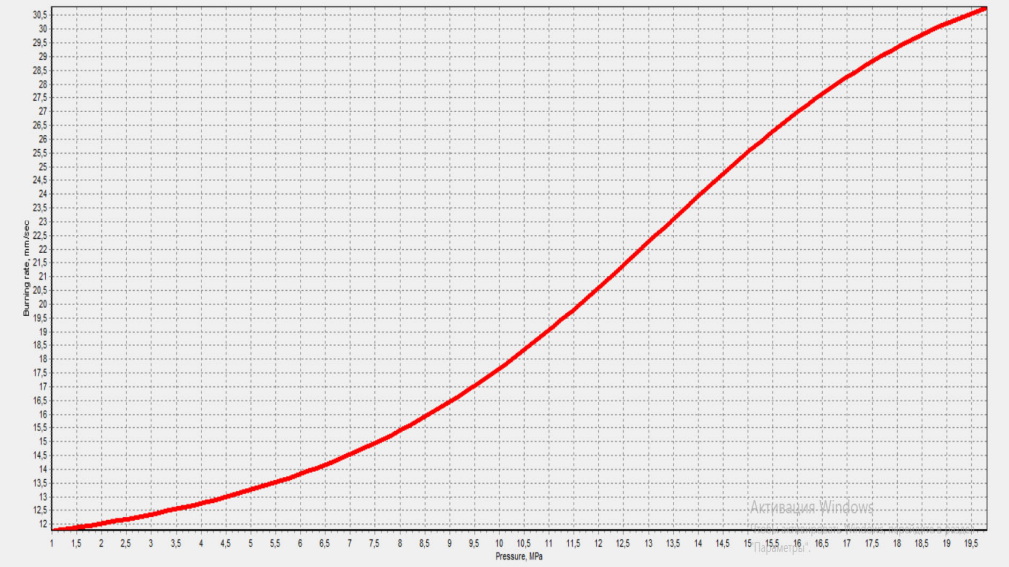
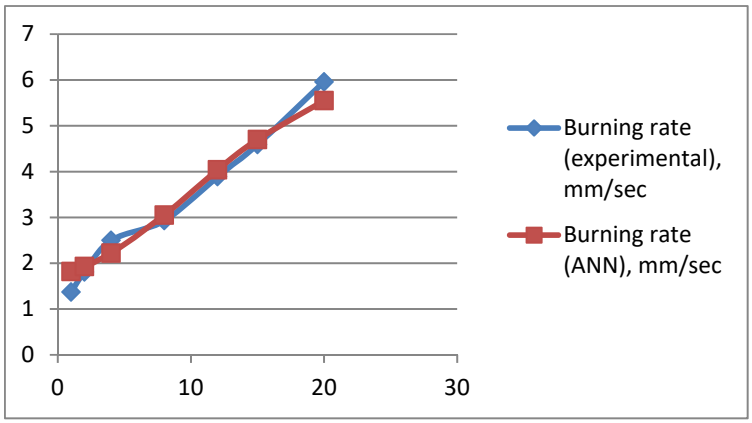


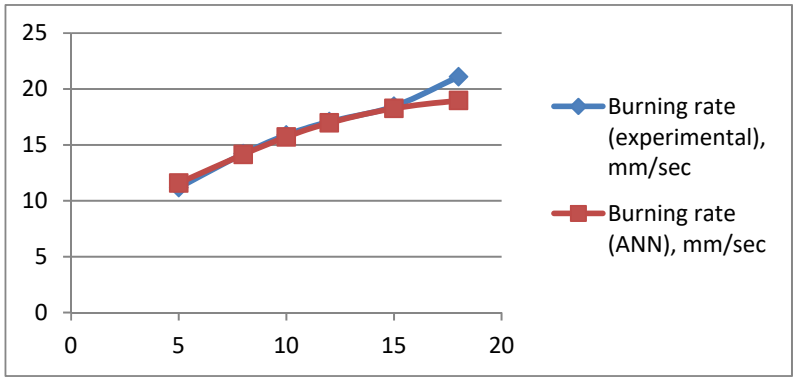
Figure 9. The graphs of the dependence of the burning rate on pressure, corresponding to the results of calculation of ANN MCM for virtual experiment (right side of the Table 3, direct task for a virtually modified propellant composition.

Pressure, MPa	Burning rate, mm/s	
	Experimental	ANN
1	1.37	1.82
2	1.81	1.93
4	2.50	2.22
8	2.93	3.05
12	3.89	4.04
15	4.59	4.70
20	5.96	5.55



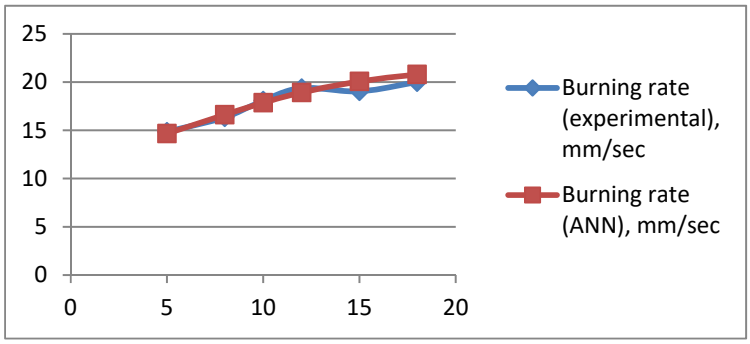
(**a**)

Pressure, MPa	Burning rate, mm/s	
	Experimental	ANN
5	11.18	11.59
8	14.21	14.15
10	15.89	15.71
12	17.08	16.97
15	18.45	18.27
18	21.10	18.97



(**b**)

Pressure, MPa	Burning rate, mm/s	
	Experimental	ANN
5	14.86	14.66
8	16.35	16.62
10	18.09	17.86
12	19.38	18.93
15	19.05	20.08
18	20.00	20.8



(**c**)

Figure 10. Comparison curves of predicted burning rate with experimental data of solid propellants. (**a**): 73.5% NG/NC + 19.5% burning rate inhibitor + 4.0% catalyst + 3.0% additives; (**b**): 63.0% NG/NC + 2.3% catalyst + 2.8% additives + 26% RDX + 4.6% diethyl phthalate (DEP) + 1.3% (nAlN); (**c**): 63.0% NG/NC + 2.3% catalyst + 2.8% additives + 26% RDX + 4.6% diethyl phthalate (DEP) + 1.3% (Al_2O_3).

5. Conclusions

1. The usage of ANN for the creation of new MCM of the propellants combustion and detonation, that solve the direct and inverse tasks as well execute the virtual experiments, depict that ANN have the wide possibilities for propellants combustion and detonation research and development of new kind of advanced propellants. The results presented in this article depict no more than 1% of the propellants combustion patterns contained in the obtained MCM.

2. The autonomous computer module of MCM allows reader to independently and in detail study all the regularities contained in the ANN model, visualizing in the form of hundreds of graphs those regularities that the authors of the article could not present in the article due to the limitations on the volume of the article. Instructions for using the executable ANN model are included with the module.
3. The autonomous computing module of MSM can be utilized. This allows researchers to calculate the values of the burning rate for energetic compositions at various conditions, visualize the patterns contained in the experimental data, conduct virtual experiments, and predict the burning rate of propellants at different pressures. The virtual experiments are a very promising means to develop new and advanced solid propellants in the framework of HEMG.

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Abbreviations

HEMG	high-energy materials genome
HEMs	high-energy materials
ANN	artificial neural networks
MCM	multifactor computational models
SRP	solid rocket propellant
NEPE	nitrate ester plasticized polyether
AI	artificial intelligence
mAl	micro-sized aluminium
nAl	nano-sized aluminium
MGI	materials genome initiative
ML	machine learning
EMGI	energetic materials genome initiative
MI	materials informatics
ICSD	inorganic crystal structure database
CHNO	carbon, hydrogen, nitrogen, and oxygen
AN	artificial neuron
RMS	root-mean-square
nNi	nano-sized nickel
RDX	hexogen
CL-20	hexanitrohexaazaisowurtzitane
CMDB	compound-modified double base
NG	nitroglycerin
NC	nitrocellulose
DEP	diethyl phthalate
Al_2O_3	aluminium trioxide
nDPN	a type of nano-sized composite
HMX	octogen
nAlN	nano-sized aluminium nitride

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