

# Application of Neural Networks for Modeling Detonation Characteristics of High-Energy Materials

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## Abstract

Machine learning methods, particularly neural networks, offer the ability to identify complex nonlinear relationships between detonation characteristics, structure, and composition of HEMs. This work employs a novel approach a cascade of neural networks to improve model quality and enable comprehensive analysis of HEM characteristics.

**Keywords:** Machine learning; Neural networks; High-energy materials; Detonation characteristics

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## Introduction

Modern challenges in the study of high-energy materials (HEMs) require effective methods for predicting performance characteristics. Traditional approaches based on experimental studies and theoretical calculations are often resource-intensive. Machine learning methods, particularly neural networks (NNs), offer the ability to identify complex nonlinear relationships between detonation characteristics, structure, and composition of HEMs [1-3]. This work employs a novel approach a cascade of neural networks to improve model quality, to obtain very smooth goal function dependences and enable comprehensive analysis of HEM characteristics.

## Materials and Methods

The study was conducted on a dataset comprising 32 individual and composite explosives. For each HEM, 7 physicochemical parameters were considered: density, oxygen balance, nitrogen content, total nitrogen and oxygen content, standard enthalpy of formation, melting point, and decomposition temperature point.

A cascade neural network method (sequential approximation) was used to predict four target variables: detonation velocity, detonation pressure, impact sensitivity, and friction sensitivity. The method proceeds as follows:

The first neural network (NN1) is trained directly on experimental data: 7 HEM descriptors are input, and one detonation characteristic is output. The values obtained from NN1 are used as output targets for training the second neural network (NN2). The third cascade level (NN3) is trained on the output data of NN2, resulting in a maximally smooth dependence. Each subsequent network uses the previous network's output as target values, equivalent to sequential filtering of high-frequency noise. The final model produces a smooth mapping with RMSE below 10<sup>-5</sup>.

For objective validation, the dataset was divided into training (80%) and test (20%) sets. Training was stopped when the minimum validation error was reached. Five-fold cross-validation confirmed stability (mean R<sup>2</sup> for detonation velocity: 0.994±0.003).

## Results and Discussion

The constructed models demonstrate high quality (Table 1).

**Table 1:** Models quality metrics.

Parameter	R <sup>2</sup>	MSE	MAE	MAPE %
Detonation velocity	0.996	0.07	0.025	0.76
Detonation pressure	0.993	0.662	0.002	0.27
Impact sensitivity	0.862	5.611	1.743	22.37
Friction sensitivity	0.877	42.35	8.624	6.92

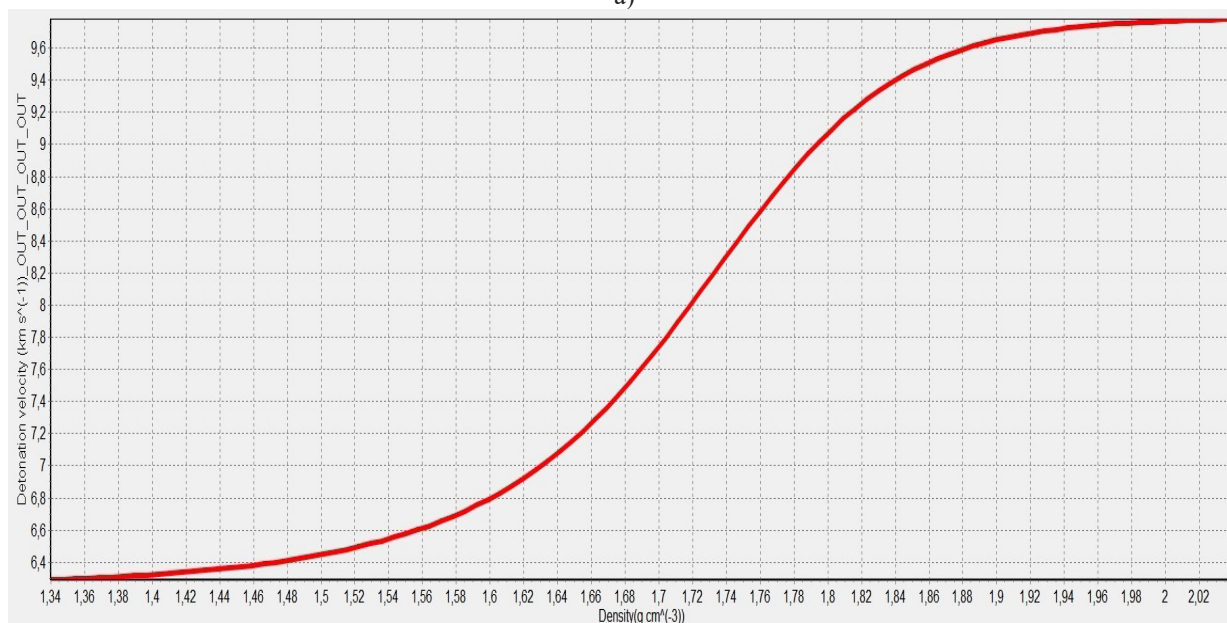
Comparison with alternative methods [4-6] shows typical R<sup>2</sup> values of ~0.95-0.99, while our cascade approach achieves R<sup>2</sup> ≈ 0.996 and 0.993 for detonation velocity and pressure, confirming

its high quality.

Analysis of physical regularities: The models reveal fundamental explosion physics: monotonic increase of detonation velocity and pressure with density (following classical detonation equations [7,8]) – Figures 1 & 2, dependence of detonation velocity on enthalpy of formation – Figure 3, dependence of detonation velocity on decomposition temperature – Figure 4, dependence of impact sensitivity on nitrogen content and decomposition temperature – Figures 5 & 6.

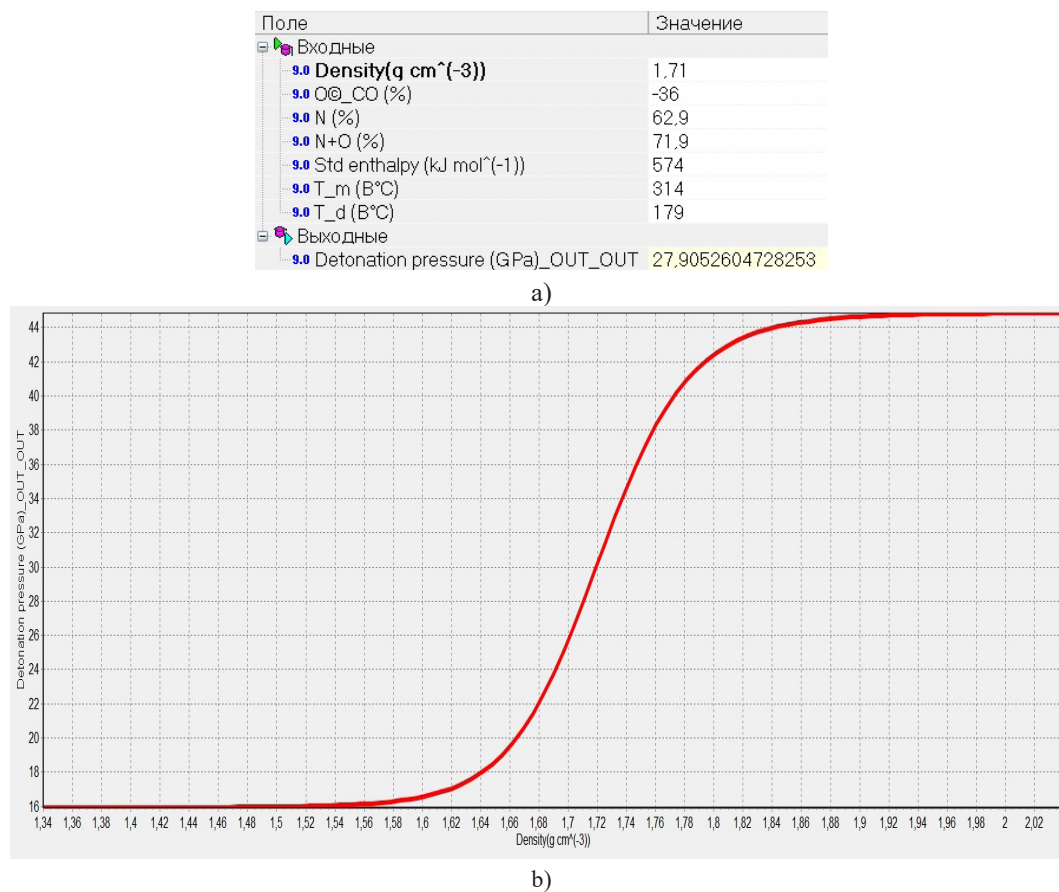
Поле	Значение
Входные	
9.0 Density(g cm <sup>-3</sup> )	1,71
9.0 O@_CO (%)	-36
9.0 N (%)	62,9
9.0 N+O (%)	71,9
9.0 Std enthalpy (kJ mol <sup>-1</sup> )	574
9.0 T_m (B°C)	314
9.0 T_d (B°C)	179
Выходные	
9.0 Detonation velocity (km s <sup>-1</sup> )_OUT_OUT_OUT_OUT	7,8784056

a)

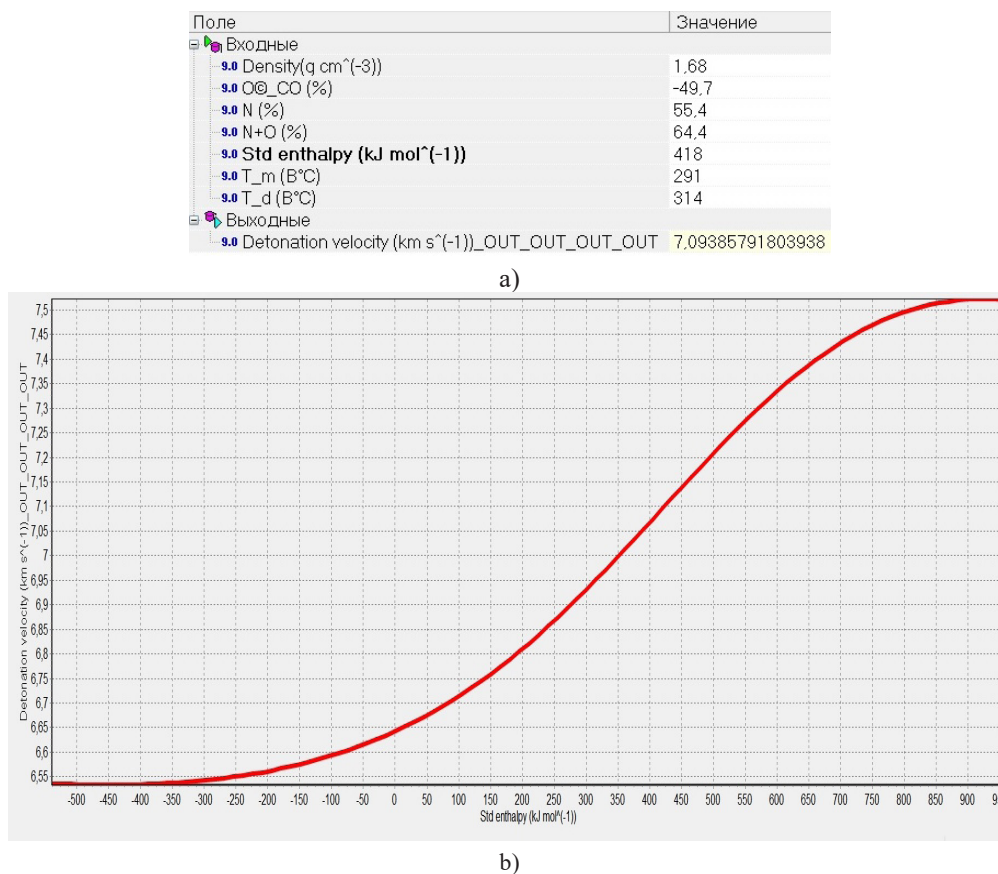


b)

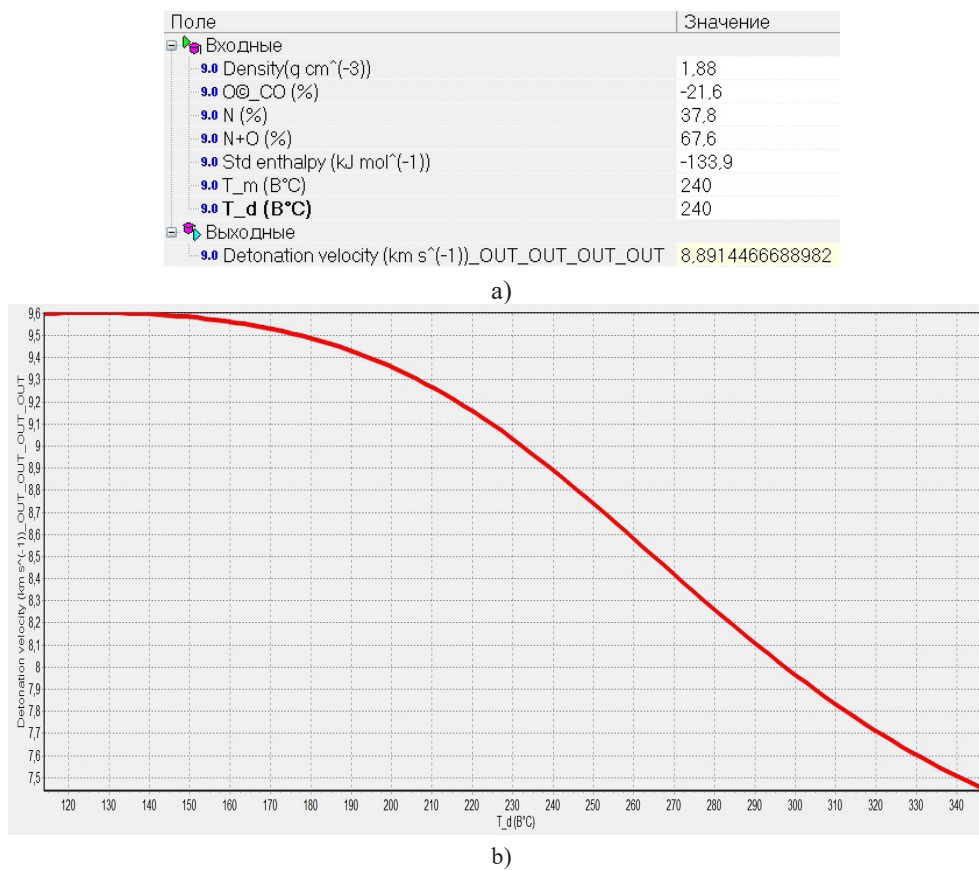
**Figure 1:** The result of calculation (a) and the dependence of detonation velocity on density (b).



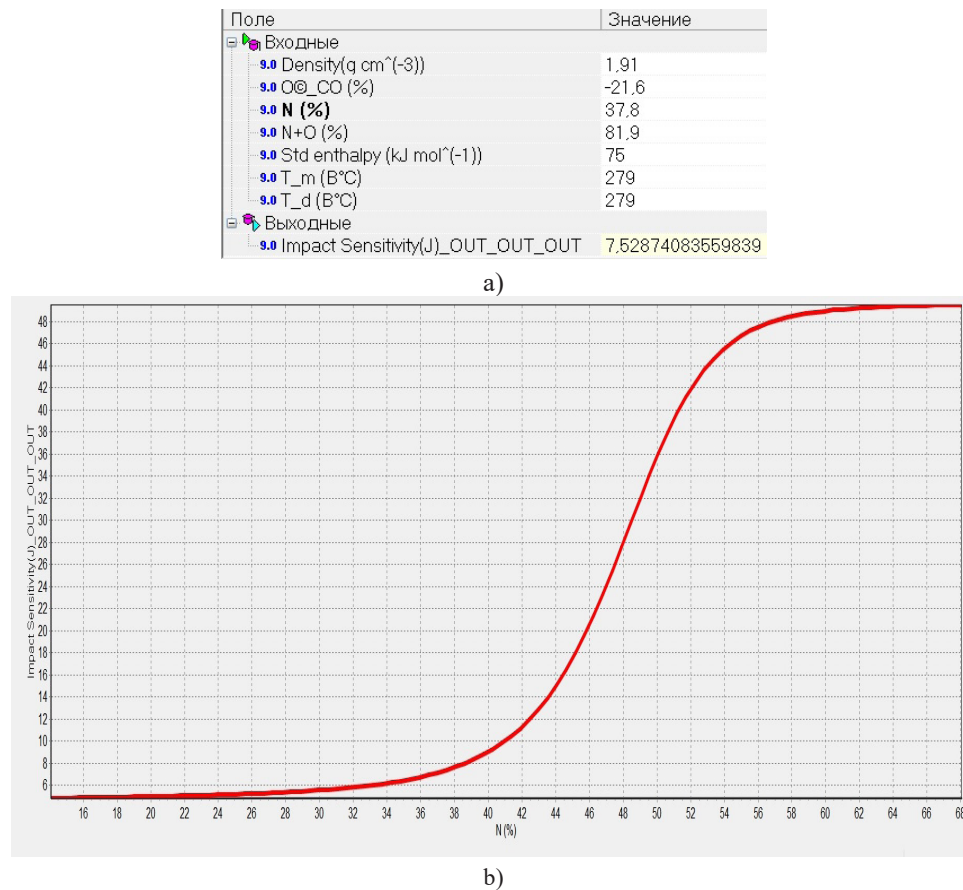
**Figure 2:** The result of calculation (a) and the dependence of detonation pressure on density (b).



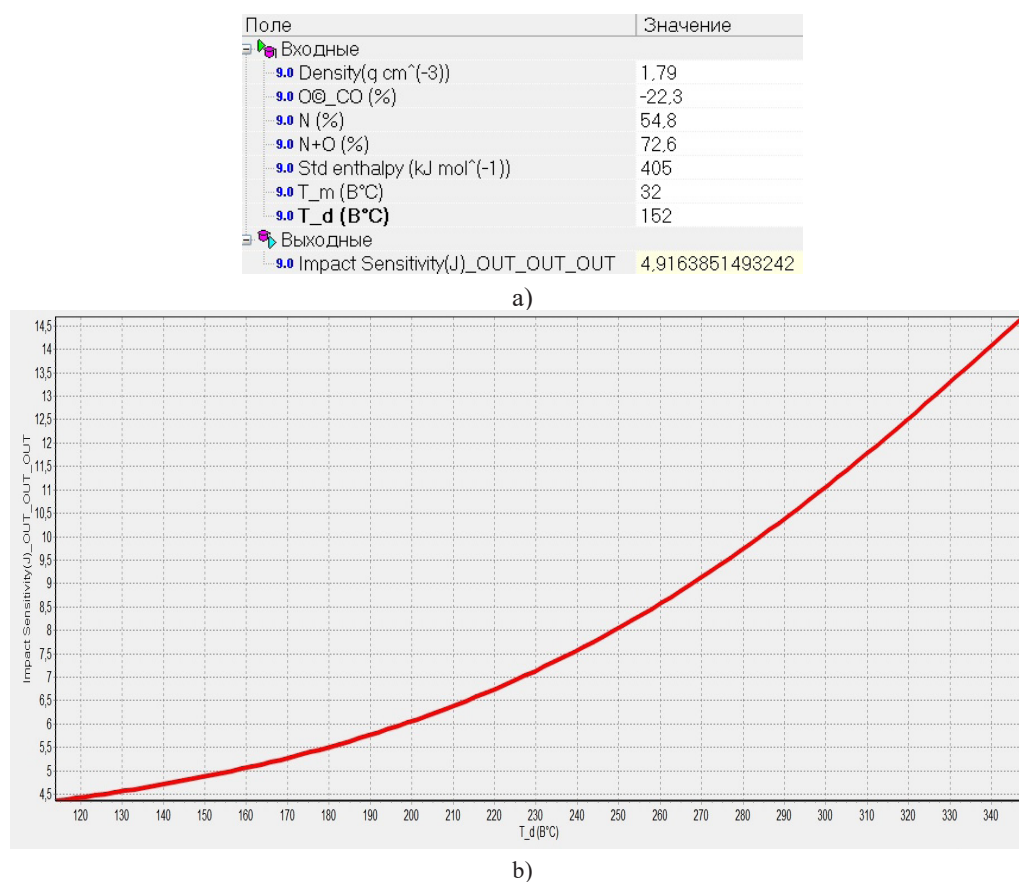
**Figure 3:** The result of calculation (a) and the dependence of detonation velocity on enthalpy of formation (b)



**Figure 4:** The result of calculation (a) and the dependence of detonation velocity on decomposition temperature (b).



**Figure 5:** The result of calculation (a) and the dependence of impact sensitivity on nitrogen content (b).



**Figure 6:** The result of calculation (a) and the dependence of impact sensitivity on decomposition temperature (b).

Analysis shows maximum influence on detonation velocity/pressure from density and oxygen balance, while sensitivity depends most on total nitrogen and oxygen content and decomposition temperature, agreeing with physicochemical concepts.

## Results and Discussion

The cascade neural network approach effectively computes HEM detonation characteristics with high accuracy ( $R^2 > 0.99$  for detonation velocity and pressure). The models adequately reflect fundamental regularities of explosive physics. For sensitivity characteristics, satisfactory results ( $R^2 > 0.86$ ) were obtained; lower accuracy is explained by measurement methodology dependence. Future work involves database expansion and creating a "High-Energy Materials Genome" [9-15].

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