APPLICATION OF A CASCADE OF NEURAL NETWORKS FOR MODELING DETONATION CHARACTERISTICS OF HIGH-ENERGETIC MATERIALS

V. S. Abrukov, D. A. Anufrieva, S. S. Kuzmin, and D. A. Sapyorov

I. N. Ulianov Chuvash State University, 15 Moskovsky Prosp., Cheboksary 428015, Russian Federation

Abstract: The paper presents the results of modeling the detonation characteristics of high-energy materials (HEMs) using a cascaded neural network method developed that ensures high modeling accuracy. Individual and composite explosives were selected as the objects of study. Four key characteristics were evaluated: detonation velocity; detonation pressure; impact sensitivity; and friction sensitivity. Seven physicochemical descriptors (namely, density, oxygen balance, nitrogen content, the sum of nitrogen and oxygen contents, standard enthalpy of formation, melting temperature, and decomposition temperature) served as the input parameters. A multilayer cascaded neural network architecture is demonstrated to enable the construction of smooth multidimensional dependences and significantly reduce the impact of random experimental errors. The main quality metrics of the models are given: determination coefficient, root-mean-square error, and mean absolute error. The neural network models are shown to adequately reproduce fundamental physical regularities, including the increase in detonation velocity and pressure with increasing density of the material. The limitations of one-dimensional slices of multifactor hypersurfaces are discussed, along with prospects for extending the database.

Keywords: high-energy materials; detonation characteristics; neural networks; multifactor computational models; cascade of neural networks; machine learning

DOI: 10.30826/CE26190310 **EDN:** GASDXF

Figure Captions

Figure 1 Comparison of experimental (*1*) and neural network calculated (*2*) detonation velocities (*a*), detonation pressures (*b*), impact sensitivities (*c*), and friction sensitivities (*d*)

Figure 2 Dependence of the detonation velocity (*a*) and detonation pressure (*b*) on the density of HEM

Figure 3 Dependence of the detonation velocity on the standard enthalpy of formation

Figure 4 Dependence of the impact sensitivity on the nitrogen content (*a*) and decomposition temperature (*b*)

Table Captions

Table 1 Initial data for the investigated individual and composite HEMs (data taken from [10–12])

Table 2 Quality metrics of the model 3

Acknowledgments

The work was partially funded by a grant from Chuvash State University (program “Young Scientists”), 2026.

References

1. Lyasheva, S. A., M. P. Shleymovich, A. P. Kirpichnikov, and A. N. Spitsin. 2015. Prognozirovanie skorosti detonatsii individual’nykh vzryvchatykh veshchestv s ispol’zovaniem neyronnoy seti [Prediction of detonation velocity of individual explosives using a neural network]. *Vestnik tekhnologicheskogo universiteta* [Herald of Technological University] 18(15):226–229.
2. Perederin, Yu. V., and N. I. Popok. 2019. Kolichestvennyy analiz i prognozirovanie svoystv komponentov energeticheskikh kondensirovannykh sistem — brizantnykh vzryvchatykh veshchestv [Quantitative analysis and prediction of properties of components of energetic condensed systems — high explosives]. *Khimicheskaya fizika i mezoskopiya* [Chemical Physics and Mesoscopy] 21(2):245–253.
3. Mukhutdinov, A. R., M. G. Efimov, and Z. R. Vakhidova. 2021. Neyrosetevoe modelirovanie protsessa detonatsii smesi geksida s inertnymi napolnitelyami [Neural network modeling of the detonation process of a mixture of hexogen with inert fillers]. *Informatsionnye tekhnologii i vychislitel’nye sistemy* [Information Technologies and Computing Systems] 4:83–90. doi: 10.14357/20718632210408.
4. Abrukov, S. V., E. V. Karlovich, V. N. Afanasyev, Y. V. Semenov, and V. Abrukov. 2010. Creation of propellant combustion models by means of data mining tools. *Int. J. Energetic Materials Chemical Propulsion* 9(5):415–432.

5. Abrukov, V. S., A. V. Kochergin, and D. A. Anufrieva. 2016. Iskusstvennye neyronnye seti kak sredstvo obobshcheniya eksperimental'nykh dannykh [Artificial neural networks as a tool for generalization of experimental data]. *Vestnik Chuvashskogo universiteta* [Bulletin of Chuvash University] 3:155–162.
6. Chandrasekaran, N., C. Oommen, V. S. Kumar, A. N. Lukin, V. S. Abrukov, and D. A. Anufrieva. 2019. Prediction of detonation velocity and N–O composition of high energy C–H–N–O explosives by means of artificial neural networks. *Propell. Explos. Pyrot.* 44(5):579–587.
7. Pang, W., V. Abrukov, D. Anufrieva, and D. Chen. 2023. Burning rate prediction of solid rocket propellant (SRP) with high-energy materials genome (HEMG). *Crystals* 13(2):237–252.
8. Anufrieva, D., V. Abrukov, V. Bozic, and D. Sapyorov. 2025. Determination of combustion law parameters based on noisy experimental data. *15th Workshop (International) on Combustion and Propulsion Advanced Design, Additive Manufacturing, and Characterization of Modern Energetic Materials: Book of Abstracts*. Pescara, Italy. 26.
9. Anufrieva, D., V. Abrukov, V. Bozic, and D. Sapyorov. 2025. Determination of combustion law parameters from noisy experimental data using a novel sequential neural network approach. *16th Symposium (International) on Combustion and Plasma Chemistry. Physics and Chemistry of Carbon and Nanoenergetic Materials: Book of Abstracts*. Almaty: Institute of Combustion Problems. 33–36.
10. Smith, J., L. Johnson, K. Brown, *et al.* 2015. Experimental and theoretical study of detonation parameters for novel energetic composites. *Org. Lett.* 17:1234–1238. doi: 10.1021/acs.orglett.5c03057.
11. Yelemessova, Zh., B. Milikhat, A. Yerken, Z. Mansurov, and A. Imangazy. 2025. Energetic composite materials for micro initiation systems: Composition-performance relationships. *Chemical J. Kazakhstan* 2(90):62–80. doi: 10.51580/2025-2.2710-1185.23.
12. Yu, J., S. Xu, W. Pang, H. Jiang, and Z. Zhang. 2025. The structural regulation and properties of energetic materials: A review. *Nanomaterials* 15(15):1140. doi: 10.3390/nano15151140.
13. Klapötke, T. M., S. Cudziło, and W. A. Trzciński. 2021. An answer to the question about the energetic performance of TKX-50. *Propell. Explos. Pyrot.* 47(6):e202100358. doi: 10.1002/prep.202100358.
14. Elton, D., Z. Boukouvalas, M. Butrico, *et al.* 2018. Applying machine learning techniques to predict the properties of energetic materials. *Sci. Rep. — U.K.* 8:9059. doi: 10.1038/s41598-018-27344-x.
15. Elton, D., Z. Boukouvalas, M. Fuge, *et al.* 2019. Deep learning for molecular design — a review of the state of the art. *Molecular Systems Design Engineering* 4:828–849. doi: 10.1039/C9ME00039A.
16. Liu, W. H., Q. J. Liu, F. S. Liu, *et al.* 2025. Machine learning approaches for predicting impact sensitivity and detonation performances of energetic materials. *J. Energy Chem.* 102:161–171. doi: 10.1016/j.jechem.2024.10.035.
17. Zel'dovich, Ya. B., and Yu. P. Raizer. 1967. *Physics of shock waves and high-temperature hydrodynamic phenomena*. New York, NY: Academic Press. 2 vols. 944 p.
18. Fickett, W., and W. C. Davis. 2000. *Detonation: Theory and experiment*. Mineola, NY: Dover Publications. 416 p.
19. Klapötke, T. M. 2018. *Energetic materials encyclopedia*. Berlin: de Gruyter. 521 p.
20. Klapötke, T. M. 2025. *Chemistry of high-energy materials: Explosives, propellants, pyrotechnics*. Walter de Gruyter GmbH & Co KG. 631 p.

Received December 1, 2025
After revision April 15, 2026
Accepted April 20, 2026

Contributors

Abrukov Viktor S. (b. 1952) — Doctor of Science in physics and mathematics, professor, head of department, I. N. Ulianov Chuvash State University, 15 Moskovsky Prosp., Cheboksary 428015, Russian Federation; abrukov@yandex.ru

Anufrieva Darya A. (b. 1986) — senior lecturer, I. N. Ulianov Chuvash State University, 15 Moskovsky Prosp., Cheboksary 428015, Russian Federation; kafedra.pfn@mail.ru

Kuzmin Sergey S. (b. 2000) — postgraduate student, I. N. Ulianov Chuvash State University, 15 Moskovsky Prosp., Cheboksary 428015, Russian Federation; sergei.kuzmin.student@yandex.ru

Sapyorov Daniil A. (b. 1999) — postgraduate student, I. N. Ulianov Chuvash State University, 15 Moskovsky Prosp., Cheboksary 428015, Russian Federation; daniil.sapyorov@mail.ru