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Opinion

From the Energetic Materials Genome to the Drugs Genome

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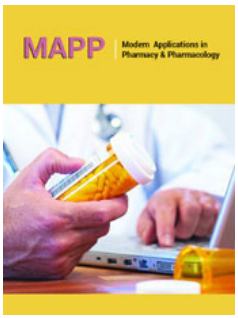

Annotation

The capabilities of multifactor computational models of experimental data enriched with metadata in the field of combustion and detonation of energetic materials with complex chemical composition are described. Models created using neural networks allow for solving direct and inverse problems, conducting virtual experiments, and solving prediction tasks. The collection of such models implements the concept of the "Genome of Energetic Materials". The prospects for creating similar models in pharmacology and setting tasks for creating a Drugs Genome are demonstrated.

Keywords: Genome; Experimental data; Neural networks; Multifactor computational models; Energetic materials; Drug compounds

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Opinion

There is a very large amount of experimental data on the characteristics of combustion and detonation of chemically complex Energetic Materials (EM). Obviously, the characteristics of combustion and detonation are related to the chemical composition of the EM components, the type of catalytic and other additives, and other EM parameters. However, at present, there are no generalized Multifactorial Computational Models (MCMs) for predicting the effect of these parameters on the rate of combustion or detonation of new EM compositions under various conditions (direct problem). There are no MVMs that make it possible to determine the chemical composition of the EM required to achieve the desired burning or detonation rate (the inverse problem). Therefore, it is necessary to carry out a large number of expensive and dangerous experiments in order to obtain a new composition of EM with desired characteristics.

This paper describes the results of using Artificial Neural Networks (ANNs) [1-4] to create generalized MCM connections between various factors and target functions (burning rate and detonation rate), which solve direct and inverse problems, and also allow you to conduct virtual experiments and solve forecasting problems. The combination of such MCMs makes it possible to implement the concept of the "Energetic Materials Genome" (EMG). By EMG, the authors mean a set of MCMs containing relationships between all variables of the combustion and detonation process of EM, which make it possible to determine the EM composition that provides the required combustion rate at a given pressure and initial temperature, the parameters of the "burning law", the temperature sensitivity of the burning rate, the detonation rate and sensitivity to external influences.

The EMG is based on data on the burning rate, detonation rate, and sensitivity to external influences of the most diverse chemical composition of energy materials (solid and liquid) under various conditions. Figure 1 presents, as an example of one of the many possibilities of ANN, the results of solving the inverse problem of detonation-determining which composition of the EM molecule provides the required detonation velocity [1]. The situation that has developed in the field of EM exists in pharmacology and pharmacy. There is also an extremely large amount of very diverse data on drug compounds and biologically active molecules accumulated here. Therefore, the use of ANN to generalize available data, predict the physic-chemical and biological characteristics of promising chemical compounds, their toxicological and biological activity, the development of new drug compounds and materials

can be considered as a very promising area of research, including from the point of view of setting the task of creating a "Drags Genome". The first steps in the implementation of this concept can be done by limiting the range of tasks to be solved to a specific area of pharmacology and a specific class of chemical compounds. In particular, the generation of new drug-like molecules is an important task.

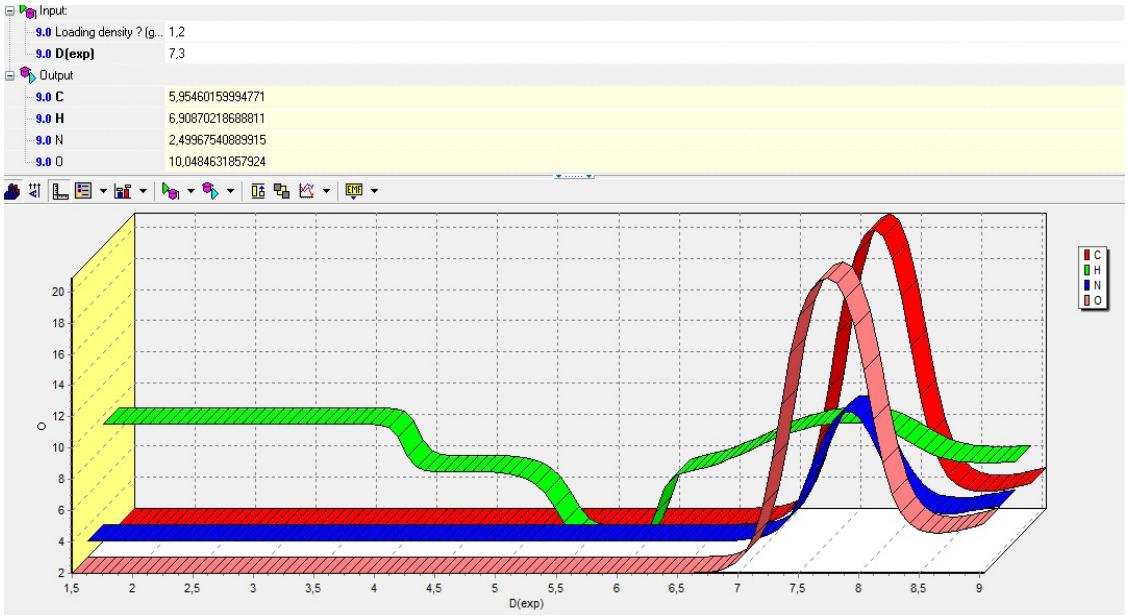

Figure 1: The results of calculating the number of C, H, N and O atoms in an EM molecule that provides the required detonation rate at a given density (see the Table above the graphs). The graphs show changes in the required number of C, H, N and O atoms in the EM molecule depending on the value of the detonation velocity, at a fixed value of the EM density.

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