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NEURAL NETWORK MODELING OF PLASMA-CHEMICAL PROCESSES OF OBTAINING NANOSYSTEMS

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Abstract. Plasma-chemical technology is a new area of industrial chemical technology. Chemical processes in low-temperature plasma, the regularities of reactions, and the basis of plasma-chemical technology will require computer simulation. Building adequate simulation models of plasma-chemical processes for developing nanosystems and computer simulations with them allows the development of applied research studies in this subject area. Computer intelligence technologies provide an opportunity to use non-classical approaches to building mathematical models of chemical processes. Neural network technologies make it possible to create mathematical simulation models of various processes.

Keywords: neural networks, neural network modeling, plasma-chemical processes, nanosystems.

Nanosystems of different compositions and organizations are currently widely studied in the course of improvement of synthesis methods according to the requirements of the present with the possibility of obligatory forecasting and management of functional properties for further application in different spheres. It is predicted that the global market value of nanotechnology will reach more than $90 billion by 2023 [1], as consumer and industrial use of nanostructures is constantly increasing.

From the nano industry perspective direction, which meet modern requirements are plasmoridine methods of synthesis of different configurations [2]. The latter, due to the possibility of different configurations and technological parameters, allows the synthesis of nanosystems of different compositions and structures. Despite significant experimental and theoretical research physio-chemical processes are complex and not completely learned for scale-up and their control in serial production. Therefore, the question of computer modeling of plasma-chemical synthesis is topical.

Construction of adequate simulation models of plasma-chemical processes of nanosystems and computer modeling with them allow solving application problems in this subject area. Modeling of processes in a liquid under the influence of plasma is complex and requires an understanding of the complex influence of processes and liquids and on the boundary of the distribution of phases "liquid-plasma".

Technologies of computing intelligence provide an opportunity to use non-classical approaches to the construction of mathematical models of chemical processes. Neuro networking technologies allow the creation of mathematical simulation models of different processes [3, 4]. Modeling of plasma chemical processes, and nanosystems including, using neural networks (NN) allows us to build implicit mathematical models and conduct experiments with them. The application of artificial intelligence systems allows for solving problems, even when traditional approaches cannot be applied for different reasons. The advantage of this approach is that the trained NN can be used for modeling.

For physiochemical processes of nanosystems, in particular: The superfine plasma range for nanosystems of noble metals (gold, silver), it is proposed to carry out neural network modeling.

Numerous experiments of nanosystems reception in physiochemical processes have been carried out repeatedly, therefore these results are offered to formalize the application of NN.

As an architecture NN is considered a multilayer neural network with sigmoid activation functions. The number of layers varies from one to three. As an algorithm of neural network learning, a well-known algorithm of inverse propagation of an error [4, 5] is used.

The input parameters of NN are: the concentration of the AgNO3 precursor (0,5-3,0 mmol/l); the type of stabilizer in the system, which determines the functionality of nanoparticles and, as a result, the sphere of practical use (sodium citrate, sodium alginate, polyvinyl alcohol, and others); duration of the plasma range (0,5-7,0 min). The plasma range is characterized by the force of current (120-220 mA with step 10 mA), voltage (6000-8000 V), and pressure of gas phase (0,6-0,8 MPa with step 0,1 MPa).

The output parameters for the NN for controlled synthesis of nanosystems are: the size of nanoparticles received (fluctuations can occur within 1-100 nm); the polydisperse index (IPD) (0,5-1,0 – polydisperse medium, 0,02-0,5-monopdisperse medium); zeta-potential (mV) – aggregate stability of nanoparticles (30 mV and above, or - 30. The description of NN architecture can be considered complete.

As is known, a separate stage of NN training is the preparation of the educational selection, i.e. at the previous stage the analysis of input data was carried out. The success of network training depends on its quality. At this stage, we removed "noisy" samples and those that are repeated, i.e. samples that are not informative. The error of NN training is proportional to the volume of the educational sample [5]. When filling the training selection with new samples in the work in the implemented software, the addition of the NN is provided.

The results of numerous experiments give an opportunity to assert that the trained NN model is well able to generalize the samples of the educational selection, which were reserved for testing, so the process of studying the NN can be considered successfully completed. The advantage of this approach is that for computer modeling of plasma-chemical processes of nanomaterials reception, a created and taught neuro boundary model can be used.

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