The use of neural networks for modeling the thermophysical characteristics of epoxy composites treated with electric spark water hammer

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Abstract
In this work, the properties of epoxy composites modified with an active plasticizer were modeled. The material was treated with electrospark water hammer. The material was treated with electric spark water hammer, which improves their physical and mechanical properties. The main attention is paid to the study of the thermal coefficient of linear expansion, which is a critical parameter for the use of composites in different temperature conditions. The results of modeling the thermophysical characteristics showed a high correlation with the experimental data, where the correlation coefficient in the test sample was 0.99%. The prediction error of epoxy polymers filled with DEG-1, aluminum oxide, chromium oxide, and carbon black by neural networks is 0.11, 0.17, 0.93, and 0.04% in test samples for different fillers. It has been shown that neural networks are capable of analyzing data and learning from it. Therefore, modeling the properties of materials by neural networks allows achieving high prediction accuracy.

Keywords
Machine learning, neural networks, composite

1. Introduction

The development of modern industry raises the problem of using new materials with predetermined characteristics. In this area of research, the use of automation systems for research processes is promising when creating such materials. The use of automated systems, namely, neural networks [1, 2], creates conditions for predicting and targeted regulation of the performance characteristics of materials. Neural networks are used in

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research to predict the properties and process the experimental results obtained for polymer composites containing various additives [3, 4]. It is known [5, 6] that machine learning uses intelligent data analysis with the ability to build a meaningful relationship between the results of experiments in the system "material composition - properties". In particular, this approach is effective in the study of polymeric composite materials based on reactoplastics. An epoxy diane binder was used in the successful cutout. It should be emphasized that the accuracy of the systems depends on the selected parameters of neural networks [7]. In general, the properties of polymer composites are modeled with great accuracy using machine learning algorithms, namely, neural networks. The advantage of this approach is the possibility of obtaining research results by the proposed method of non-destructive testing without its effect on changes in the structure of the epoxy composite.

The modern technology of creating polymer composites, including epoxy composites, is aimed at studying methods of controlled directed changes in the material structure parameters. The latter, in most cases, determine the physical, mechanical, and operational characteristics of epoxy composites [8-11]. This approach is based on theoretical concepts of structure formation processes and analysis of empirical data on the performance properties of the developed materials. To obtain composites with optimal characteristics, a set of requirements for the polymer matrix is established, such as high physical, mechanical, adhesive, and thermal characteristics, as well as the necessary rheological properties. This is achieved through the selection of ingredients in the polymer binder, such as modifiers, plasticizers, catalysts, and fillers [12-17]. In addition, one of the promising areas for improving the properties of heterogeneous composite systems at the present stage of development of materials science is the modification of compositions using external force fields: electromagnetic, ultrasonic, ultraviolet, and electrospark water hammer [18]. The technology of activation of oligomeric compositions by these fields at the initial stages of material formation opens up new opportunities for scientifically directed regulation of the processes of interaction between components. The possibility of adjusting the structure parameters for the targeted creation of epoxy composite materials with predetermined performance characteristics has been proven.

Polymer composite materials are used in various industries: mechanical engineering, construction, automotive, and aviation. Composite materials are increasingly used in critical elements of aircraft and automobiles. They are also used as protective coatings in oil and pumping units due to their high physical, mechanical, thermal and corrosion properties. However, to realize the potential properties of composite epoxy materials, it is necessary to use fillers, plasticizers, and modify the epoxy matrix itself with force fields. In particular, obtaining composites with high technological and operational characteristics is based on ensuring a strong and stable bond between the active centers on the surface of the filler and the macromolecules of the binder [8, 12]. It is known that the parameters of the thermal coefficient of linear expansion (TCLE) of polymers in the region of their glass transition temperature depend on the rate of temperature change.

In connection with the above, the use of neural networks in the study of TCLE, which is an important property of the thermal characteristics of epoxy composites, is an urgent problem of modern materials science.

The article [19] gives the results of the study of qualitative neural networks, including discrete and distributed time delays. A method for calculating the exponential decay rate for a neural network model based on differential equations with a discrete delay was developed and applied [20, 21].

When studying the properties of thermomechanical characteristics of epoxy composites, important characteristics of converters are taken into account [22, 23], the main of which is stability [24, 25]. Scientific studies [26] and [27] give examples of sensor response modelling. Numerical modelling in cyber-physical sensor systems [28, 29] is important at the stage of their design.

However, insufficient attention has been paid to modeling the thermal and physical characteristics of neural networks. It is important to study the materials at different temperatures of plasticized epoxy composites filled with DEG-1, aluminum oxide, chromium oxide, and carbon black using neural networks.

2. Method of research by neural networks

Neural networks are one of the most widespread machine learning methods. In particular, the prerequisite for their emergence was the study of the human nervous system. In general, a neural network is a system with a large number of neurons that can approximate rather complex dependencies and find patterns between input and output data [30]. It is known that each neuron communicates with the other through axons and synapses to process the received data and perform appropriate actions. Therefore, to simulate such a process, a perceptron is used, i.e., an artificial neuron that receives several inputs and produces one output (Fig. 1).

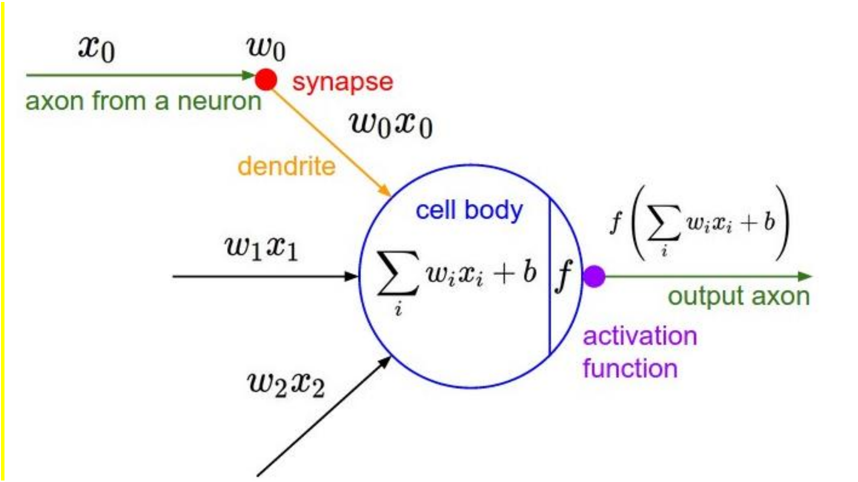

Figure 1: Model of an artificial neuron [5].

To achieve the minimum error in a neural network, it is necessary to adjust the weights between neurons [31]. That is, you need to find a set of parameters that most accurately reflects the real data distribution.

The back-propagation method is a way to adjust the weights so that the neural network produces a smaller error on training examples. Therefore, iteration after iteration, feeding the neural network with example after example and adjusting the weights, it is necessary to bring the connection vector closer to a state in which the data is obtained that meets expectations.

In general, the main parameters affecting the training process are the step size, methods of changing the step, and the method of initializing the initial values of the weights in the network. In addition, when building neural networks, it is important to choose the architecture, learning algorithm, error function, activation function of the hidden and output layers [32, 33]. The neural network training stop parameter is 1000 epochs.

In particular, in this study, such networks were built as MLP 2-10-1, for composites filled with DEG-1 and carbon black, respectively, MLP 2-8-1 for aluminum oxide and chromium oxide. The learning algorithm was BFGS, the error function was SOS, and the hidden layer activation functions were logarithmic for all fillers. Whereas the activation function of the original layer was logarithmic, and for the filler with aluminum oxide - tangential [34, 35].

3. Experimental approach

The introduction into the epoxy oligomer (ED-20), as a plasticizer, of the aliphatic resin DEG-1, which is chemically inert to the binder, but participates in the structural organization of the "sol in gel" matrix. In the process of crosslinking such a two-component system, an increase in the molecular weight of the components and gelling is accompanied by a change in the compatibility of the ingredients and, as a result, leads to the separation of the system into phases. In this case, it was assumed that the supramolecular structure of chains of aliphatic oligomer is formed in the mesh structure of the crosslinked material. The existence of globular structures of the aliphatic resin DEG-1 in the form of inclusions in the glassy epoxy mesh was established by electron microscopy. At the same time, such inclusions can be in both glassy and viscous states depending on the polymerization conditions.

It should be noted that the processes of phase separation in such two-component systems are accompanied by a change in physical properties, in particular, volumetric shrinkage, due to a decrease in the free volume in the epoxy composite material. At the same time, the gelation viscosity of the compositions is significantly reduced due to a decrease in the number of physical bonds between the macromolecules of the original epoxy oligomer. However, during polymerization, filling the free volume of the system with plasticizer molecules and, accordingly, independent crosslinking of the two-phase system leads to an improvement in the cohesive characteristics of the composite material (CM), which is confirmed by thermophysical and physicomechanical studies. The main factor in improving these characteristics is, first of all, the compatibility of the matrix components. If the considered mechanism is correct, then the improvement of the above properties should also be expected as a result of modification of the matrix components by electric spark water hammer (ESWH).

The first stage of the research was to study its effect on the physical, mechanical and thermal properties of heterogeneous materials during arc discharge treatment of matrix components. Experimentally, it was found that an excessive amount of plasticizer in the matrix, i.e. sol fraction, which is in a viscous-fluid state, significantly reduces the degree of crosslinking of the matrix. In addition, dilatometric studies have shown that the thermal coefficient of linear expansion of TCLE composites at different temperature ranges varies in the range of 293...433 K. TCLE was calculated from the curve of relative strain versus temperature, approximating this dependence with an exponential function. It is shown that the TCLE of composites with modified epoxy resin compared to a CM containing the original ED-20 is an order of magnitude lower, regardless of the concentration of the plasticizer.

It should be noted that in the temperature range of 293...383 K, a sharp decrease in the TCLE value was observed compared to other temperature ranges after the water hammer action. In this temperature range, a more significant contribution of crosslinking is realized due to the appearance of physical nodes in the spatial grid of the binder. [35, 36]. This is explained by a decrease in the strain value when the material is heated during temperature tests. We observed a decrease in the value of the thermal expansion coefficient of the TCLE. It has been experimentally established that the degree of crosslinking in the material increases [36-39]. This mechanism of TCLE reduction is confirmed by the high value of the sol fraction in the system (92-94 %). It has been proven that the yield strength of composites containing unmodified ED-20 resin in the glass transition zone is significantly higher than that of plasticized composites with a modified plasticizer. This indicates an increase in the degree of cross-linking of the matrix material after treatment with an electrohydraulic arc discharge.

It should be noted that the activity of the radicals formed during electrospark water hammering is determined by both the kinetic and thermodynamic parameters of the system. From the thermodynamic point of view, free radicals in the form of segments should be considered as active dipoles. The electric forces of both attraction and repulsion determine the behavior of active radicals when crosslinking the system. As a result, a double electric layer was observed in the system in some areas at the interface, which, in turn, significantly increases the cohesive characteristics of the material at the epoxy resin-plasticizer interface.

It was found that with an increase in temperature, the TCLE of all samples without exception also increases. Therefore, the next stage of research to reduce the TCLE was the filling of the plasticized binder with dispersed particles of aluminum oxide, chromium oxide, and carbon black. It was found that with an increase in the content of dispersed particles in the composite, the thermal coefficient of linear expansion decreases only up to certain limits. Based on this, we have determined the critical concentrations of each of the selected fillers. It has been experimentally proven that the introduction of dispersed particles at optimal concentrations (aluminum oxide 100 wt%, chromium oxides (50 wt%), carbon black (40 wt%) per 100 wt% of epoxy oligomers (hereinafter, the concentration of fillers is presented in wt. wt. % per 100 wt. % of the binder) with simultaneous pretreatment of the epoxy composite by electric spark water hammer, provides a 2.5...3.0-fold reduction in the TCLE of composites compared to the treated matrix.

The thermal coefficient of linear expansion was modeled using the experimental data obtained in [35] by neural networks. In particular, in the process of training neural networks, the data were divided into two parts - training and test samples. That is, 18,000 elements for each epoxy polymer filled with DEG-1 and carbon black, and 31,000 elements for the polymer filled with aluminum oxide and chromium oxide, respectively. Of this data, 80% was randomly selected for the training set, and the remaining 20% was left to evaluate the quality of the prediction. Here, the output parameter was the thermal coefficient of linear expansion $\alpha \cdot 10^{-5}$, K^{-1}. Filler concentration (wt%) of the plasticizer and temperature were considered as input parameters.

The dependences of the experimental data of the thermal coefficient of linear expansion on the predicted ones obtained by the neural network method are shown in Figs. 2-5.

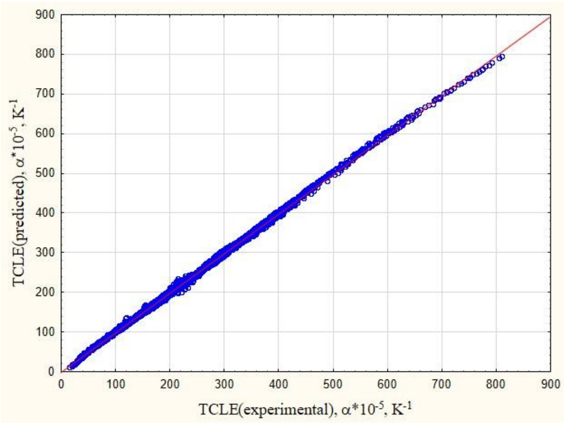

Figure 2: Predicted and experimental dependences for the composite filled with plasticizer DEG-1

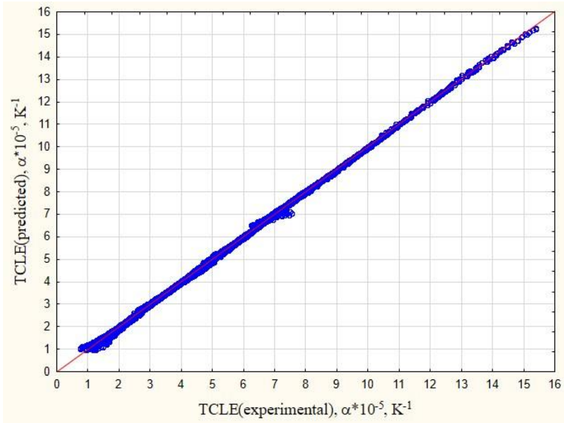

Figure 3: Predicted and experimental dependences for an aluminum oxide-filled composite

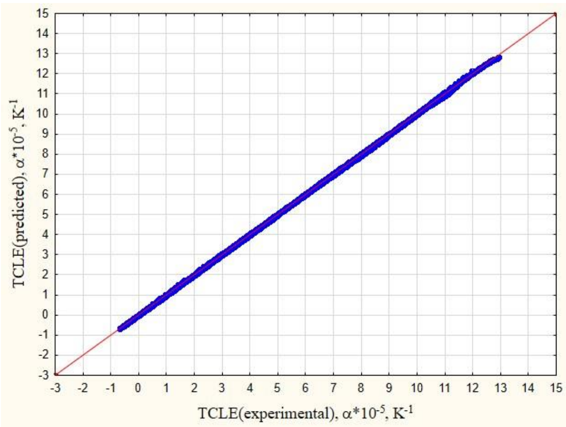

Figure 4: Predicted and experimental dependences for a chromium oxide-filled composite

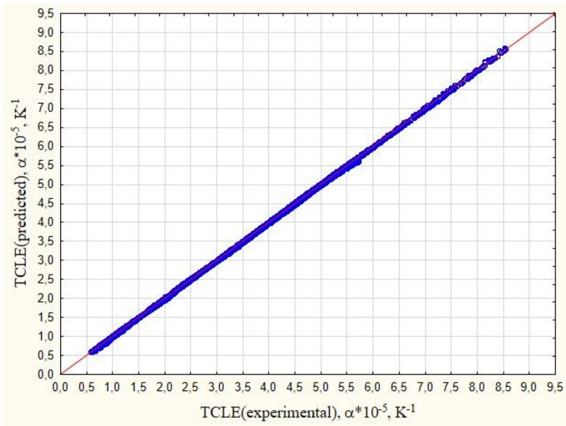

Figure 5: Predicted and experimental dependences for a composite filled with gas soot

The dependences of the predicted thermal coefficient of linear expansion on the filler concentration in the composite and temperature are shown in Figs. 6-9.

To analyze data, a statistical graph in the form of residuals diagrams is often used. It was found that the residuals have a normal distribution.

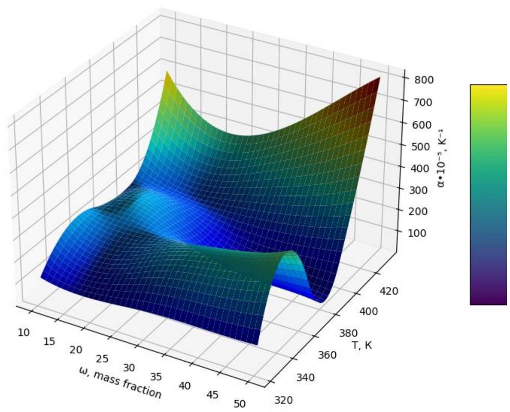

Figure 6: Temperature dependence of the thermal coefficient of linear expansion filled with DEG-1

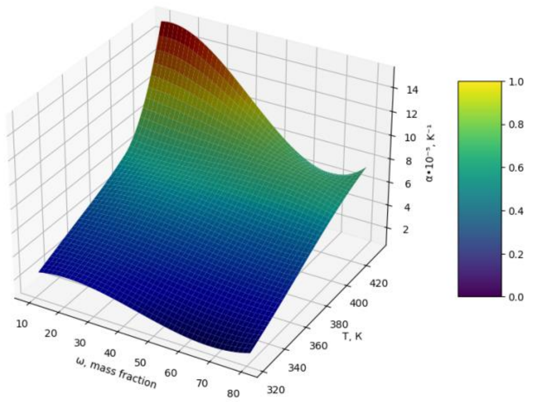

Figure 7: Temperature dependence of the thermal coefficient of linear expansion of aluminum oxide filled with aluminum oxide

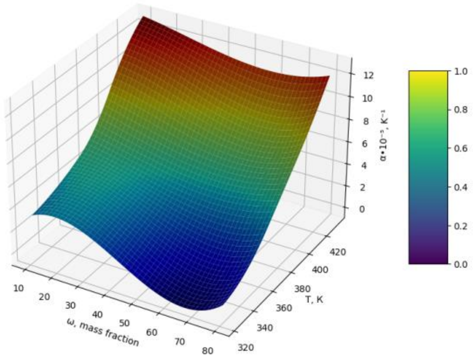

Figure 8: Temperature dependence of the thermal coefficient of linear expansion of chromium oxide filled glass

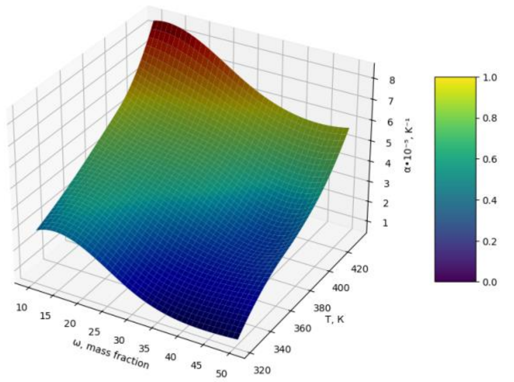

Figure 9: Temperature dependence of the thermal coefficient of linear expansion filled with carbon black

The diagrams of residual values for composites filled with DEG-1, aluminum oxide, chromium oxide, and carbon black, respectively, are shown in Figs. 10(a, b, c, d).

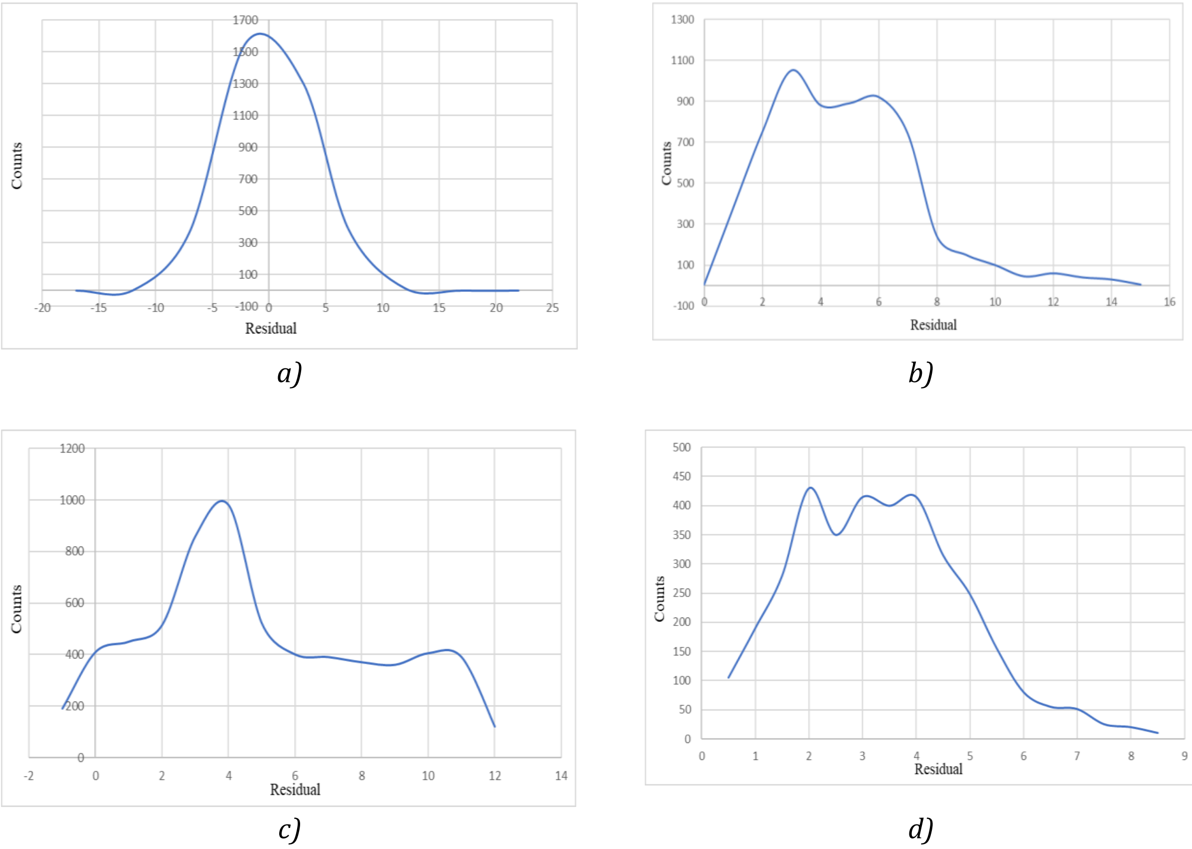

Figure 10: Diagram of residual values for composites filled with : a) DEG-1; b) aluminum oxide; c) chromium oxide; d)carbon black

4. Conclusion

The neural networks modeled the change in the thermal coefficient of linear expansion of epoxy polymers filled with DEG-1, aluminum oxide, chromium oxide, and carbon black. The results are in good agreement with the experimental data. The prediction error of the neural networks is 0.11, 0.17, 0.93, and 0.04 % in the test samples in particular, the prediction accuracy depends on such parameters as the architecture of the neural network, the activation functions of the hidden and output layers, and the learning hyperparameters. In general, optimization of each of them is critical to achieving high results. The obtained results will allow to create conditions for targeted regulation of physical and thermal characteristics by forming a structural organization in the material. The practical value of the obtained results lies in the possibility of implementing the neural network method in production processes to improve the characteristics of composite materials in various industries. Thus, the results of the study will help to increase the productivity and competitiveness of enterprises that use neural network modeling of thermal and physical characteristics in their activities. Further research is planned to optimize the processes of developing epoxy composites for various functional purposes.

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