Materials Physics and Mechanics. 2023;51(5): 66–78
Research article
http://dx.doi.org/10.18149/MPM.5152023_7

Submitted: January 27, 2023
Approved: May 23, 2023
Accepted: July 11, 2023

Prediction of mechanical properties of elastomeric materials using neural networks

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Abstract. The article is devoted to the use of neural networks for predicting the mechanical properties of rubber. Rubbers include, as a rule, more than one and a half dozen components. Each of the components has a complex and ambiguous effect on the complex of material properties. When developing new compositions, this significantly complicates and lengthens the solution of material science problems by traditional methods of composition selection. These problems can be effectively solved using machine learning techniques. The authors have developed approaches to the use of neural networks for predicting the mechanical properties of rubber from a known composition. In this article, neural network models have been created and optimized, which make it possible to predict the mechanical properties of elastomeric materials with high accuracy.

Keywords: elastomers; rubbers; physical and mechanical properties; convolutional neural network; hyperparameter optimization; neural network technologies; python language; keras library

Citation: Fomin SV, Rostovtsev VS, Meltsov VU, Shirokova ES. Prediction of mechanical properties of elastomeric materials using neural networks. *Materials Physics and Mechanics.* 2023;51(5): 66-78. DOI: 10.18149/MPM.5152023_7.

Introduction

Due to a unique set of properties – a combination of good physical and mechanical characteristics, elasticity, energy absorption ability, minimal compressibility, etc. – elastomers as structural materials are used in a large number of applications, such as seals, elements for absorbing vibrations and shocks, load-bearing structures [1,2]. The most common elastomers are rubbers, which are materials based on rubbers that acquire their operational properties as a result of the technological vulcanization of so-called raw rubber mixtures. Raw rubber compounds, in turn, are a mixture of many components. During vulcanization, individual polymer rubber molecules are “stitched” into a three-dimensional structure due to cross-links formed, most often, due to interacting with special components – vulcanizing agents. The composition of rubber compounds is very diverse and usually includes the following groups of ingredients [1,2]:

– rubber, it is an amorphous or partially crystallizing polymer, which is the basis of rubber and determines its basic set of properties;
– vulcanizing group, that is a group of components introduced into the rubber mixture to form cross-links between rubber molecules during vulcanization;
– fillers, which are a group of components introduced into the rubber mixture mainly to improve mechanical properties (reinforcing fillers), or reduce the cost (inert fillers);

Publisher: Peter the Great St. Petersburg Polytechnic University

– plasticizers, which are a group of components introduced primarily to facilitate processing of rubber compounds, as well as to expand the temperature range of rubber operation;
– age resistors, which are a group of components introduced into the composition of rubber compounds to protect them against chemical and physical aging and, accordingly, to increase the operation duration of final products;
– technological additives, which are the components introduced to facilitate technological processing of rubber mixtures;
– other components, which may provide certain narrowly specific properties. For example, components which provide electrically conductive properties of rubbers, or protect them from the effects of fire, microorganisms, etc.

To the greatest extent, the basic properties of rubbers are determined by the type of rubber, the type and content of the components of the vulcanizing group, fillers, plasticizers. At the same time, there are tens, if not hundreds, of thousands of brands of ingredients. To obtain rubbers with a given set of properties, it is necessary to correctly select the compounds of the composition – the components used and their ratio.

It should be noted that a set of characteristics of the material is significantly influenced by the conditions for obtaining rubbers. The conditions of vulcanization – temperature and duration – have the greatest influence. If vulcanization parameters are selected incorrectly, the vulcanized grid of cross-links is formed incompletely, or rubber degrades thermally. Both processes negatively affect the properties of final products.

As a rule, when developing compositions of rubber compounds with specified technological and operational characteristics, quite a lot of developer experience and accumulated empirical knowledge are required. No wonder that many professionals in rubber compounding consider their activities to be more art than engineering. It is significant that even the discovery of the rubber vulcanization itself turned out to be the result of a huge number of experiments on mixing rubber with various components. Charles Goodyear [2] spent more than ten years searching for a vulcanizing agent and, to a certain extent, accidentally discovered sulfur vulcanization. Of course, modern rubber compositions differ significantly from those used in the middle of the XIX century when C. Goodyear experimented, but empirical experience is still of great importance while obtaining the material with the specified properties.

The authors of this paper claim that problems of predicting properties of rubbers according to a known composition (a direct problem) and selecting the composition for a given set of properties (an inverse problem) can be successfully solved using modern computing.

As noted in [3], traditionally, the quantitative structure-property relationship (QSPR) model is used as a core of the descriptor model, which allows predicting properties of a material of interest based on certain input characteristics. But at the same time, the authors [3] note that it is extremely difficult to use traditional methods of linear and nonlinear correlation for these purposes due to complex relationships between inputs and outputs of the model. To predict properties, Machine Learning (ML) is much more promising.

Machine learning is a branch of Artificial Intelligence (AI). Its purpose is to create models trained on the basis of past data and situations. In recent decades, ML methods are rapidly developing due to the increased computing power of modern computers and a large amount of experimental data accumulated. ML is successfully applied to predict properties of materials in a variety of areas. Here are some examples of successful application of ML methods for materials research: predicting physical and mechanical properties of alloys [4,5], properties of inorganic materials [6], electronic forbidden zones of perovskite materials [7], catalytic activity [8,9], acid dissociation constants [10], designing organometallic sorbents [11], properties of polymer dielectrics [12], materials for producing organic light-emitting diodes (OLED) [13],

superconductors [14], photovoltaic materials [15], polymer electrolyte membranes (PEM) for fuel cells [16].

When using ML methods, it is not necessary to build complex theoretical regression models based on fundamental conservation laws and thermodynamics. In materials science, as a rule, such relations, if they exist, are extremely complicated and poorly describe the real relationship between the structure and properties. This makes it difficult to predict properties of complex materials, and it is almost impossible to solve the inverse task of selecting a composition for a given set of characteristics. However, when using ML, these difficulties almost disappear.

To solve materials science problems, when applying ML for predicting properties of materials, it is extremely important to acquire, accumulate, and systematize a large amount of experimental data to successfully train the artificial intelligence. To date, the world has accumulated a large amount of data on various materials – metals and alloys, plastics, medicines, minerals, fibers, etc. [17].

As rubbers are used to produce many critical products (e.g., automobile, aviation pneumatic tires, etc.), and their quality affects a person's life and well-being, it is necessary to predict their characteristics. Field tests are usually extremely costly, in terms of financial, labor, time, and material resources. ML methods applied can increase productivity and speed of achieving results. We have not found any research literature on the use of ML methods for predicting properties of rubbers or other elastomeric materials.

Materials and Methods

Due to the fact that more than 70 % [18,19] of the elastomers are consumed by the tire industry, the objects of the study were general-purpose rubbers traditionally used in this area: isoprene (IR, NR), butadiene (BR), styrene butadiene and methylstyrene butadiene (SBR-30). It should be noted that the proposed approach, due to its versatility, can also be extended to special-purpose elastomers: nitrile butadiene (NBR), ethylene-propylene (EPDM), fluoroelastomers (FKM) and others.

As a vulcanizing system, a combination of sulfur and sulfonamide accelerators (CBS, MBS) was used. This vulcanizing system provides optimal vulcanization kinetics: an induction period during vulcanization, which is sufficient for the composition to spread in shape; a high rate of vulcanization and a wide plateau, which makes it possible to prevent the reversion of properties.

Carbon black of various grades, dispersion, and specific surface area were used as fillers. Carbon black of the applied grades belongs to the group of reinforcing fillers that improve physical and mechanical characteristics of rubbers [1]. Some rubber mixtures contained inert fillers (chalk, kaolin, etc.) introduced to facilitate processing and reduce the cost of materials. They affected physical and mechanical properties insignificantly.

Petroleum oils were used as plasticizers: the PN-6sh petroleum plasticizer, which is a mixture of mainly aromatic hydrocarbons, paraffin oil (MP), which is a mixture of linear hydrocarbons.

These ingredients were selected due to their wide distribution, availability, convenient processing, and stable properties.

When the artificial neural network was trained, other components of rubber mixtures affected physical and mechanical properties of rubbers insignificantly.

Rubber mixtures for the control sample were prepared using laboratory mixing rollers according to the following mixing mode: rubber was plasticized; zinc oxide and stearic acid were introduced; fillers were introduced; plasticizers were introduced; components of the vulcanizing group were introduced. The mixing temperature was 60-70 °C.

Rubber mixtures were vulcanized in a hydraulic vulcanization press at 160 °C. Vulcanization lasted for 9 minutes.

To obtain a sample of input data, the results of tests of industrially produced rubbers were also used, in which samples were obtained under different conditions. This fact was taken into account when describing the input parameters.

Experimental tests of rubber properties were carried out according to the requirements of GOST 270-75. Rubber. A method for determining elastic and strength properties at elongation.

The computation was done using the MATLAB (developed by the MathWorks), as well as with the help of the program developed by the authors in the freely distributed Python programming language and ready-made libraries of this language.

Results and Discussion

Preparing data for computer modeling. In this paper, it was necessary to take into account types and contents of rubbers, the vulcanizing group, carbon black, plasticizer as input parameters (descriptors) for the neural network. The effect of the other components was considered insignificant. Obviously, it is most convenient to represent the input parameters in the form of numerical values.

The number of all components was calculated per 100 parts by weight of rubber. This made it possible to simplify the model by excluding one input parameter – rubber content, which was always equal to 100 parts by weight.

The most difficult task was to describe the structure of the ingredients used so that it could be processed on a computer. Chemists usually apply structural formulas of organic substances, for polymers, structural formulas of monomeric units are used. This is a general principle for the chemical sciences to use molecular descriptors optimized for human perception. However, the neural network required the search for numerical quantities that adequately described the structure of the components.

To describe the structure of rubbers and petroleum plasticizers, a basic thermodynamic indicator – the solubility parameter (δ) – can be used. It is fundamentally important to know solubility parameters when solving many applied problems. This parameter is often used to decide if mutual solubility of multicomponent systems [20-25], including rubber-plasticizer systems, is possible. Values of solubility parameters for various compounds, including polymers, can be found in reference books on chemical and physical and chemical properties of substances.

For low molecular weight compounds, such as petroleum plasticizers, the solubility parameter can be determined experimentally [26]. In this case, it is calculated as follows:

$$\delta^2 = \frac{\Delta E_0}{V}, \quad (1)$$

where $\Delta E_0 = \Delta H_0 - RT$ is the evaporation energy, ΔH_0 is the latent heat of the liquid evaporation, R is the gas constant, T is the absolute temperature, V is the molar volume.

For polymers, the δ parameter is difficult to determine experimentally since it is impossible to experimentally determine their evaporation energy: polymers cannot be converted to a gaseous state without being decomposed. For polymers, solubility parameters are determined based on the maximum swelling in a group of solvents with the known solubility parameter, using the results of indirect measurements [27], or computational schemes [28-31].

In this paper, the solubility parameters for petroleum plasticizers and for rubbers were obtained by computation using the method of group contributions according to the method described in [28].

In addition, for rubber, an important factor affecting physical and mechanical properties of rubbers is its ability to crystallize: the higher the degree of crystallinity, the higher the physical and mechanical parameters. In this research, it was assumed that the fraction of the crystalline phase is constant since the samples for testing were obtained under standard

conditions. Considering this, the ability of rubbers to crystallize was described by a binary input parameter taking either "1" (for rubbers that can crystallize) or "0" (for rubbers that cannot crystallize) value.

For carbon black, the iodine number was used as a numerical value characterizing its properties. This parameter, numerically equal to the amount of iodine adsorbed by carbon black, characterizes the surface of carbon black particles. The iodine number is determined according to GOST ISO 1304-2013 Ingredients of rubber mixtures. Carbon black. Determining the iodine adsorption value.

Vulcanization process parameters – temperature and duration – are numerical values. As input parameters of the model, they were used unchanged.

Thus, taking into account the above, a list of input parameters that characterize the composition of rubbers and, accordingly, affect the structure and properties of the material was formed. The list is given below (Table 1).

Table 1. List of input parameters for computer modeling

Component in rubber compound	Input parameter			
	Name	Measurement unit	Variable type	Notation
Rubber	Rubber (rubber mixture) solubility parameter	$\frac{J^{1/2}}{m^{3/2}}$	Numerical	Input1
	Rubber crystallization capacity	-	Binary	Input2
Vulcanizing group	Content of vulcanizing agent	Part by weight per 100 parts by weight of rubber	Numerical	Input3
	Content of vulcanization accelerator	Part by weight per 100 parts by weight of rubber	Numerical	Input4
Filler	Content of carbon black	Part by weight per 100 parts by weight of rubber	Numerical	Input5
	Iodine number of carbon black	$\frac{\text{mg of iodine}}{g}$	Numerical	Input6
Plasticizer	Content of plasticizer	Part by weight per 100 parts by weight of rubber	Numerical	Input7
	Plasticizer (mixture of plasticizers) solubility parameter	$\frac{J^{1/2}}{m^{3/2}}$	Numerical	Input8
Process parameters	Vulcanization temperature	°C	Numerical	Input9
	Vulcanization time	Min.	Numerical	Input10

Setting the output parameters of rubber. As previously noted, physical and mechanical properties of rubbers were used as output parameters. From a large variety, it was necessary to identify those characteristics that would be important from the point of view of operational properties of elastomeric materials, easy to determine and give a relatively low error, and would correlate with changes in input parameters well. The list of output parameters is given below (Table 2).

Table 2. List of output parameters for modeling

Rubber properties	Measurement unit	Parameter notation
Tensile strength	MPa	Output1
Stress at 300 % elongation	MPa	Output2
Elongation at break	%	Output3

Results of neural network modeling. The computer modeling scheme is presented below (Fig. 1). Rubber samples with various types of rubber, fillers, and component contents were manufactured and tested. The total number of examined samples was 36. In addition, data on the compositions of industrially produced rubbers were processed, which made it possible to obtain 84 samples. Such a sample size is insufficient for training a neural network. At the same time, many sources (e.g., [17]) note the importance of obtaining correct, accurate, and sufficient data.

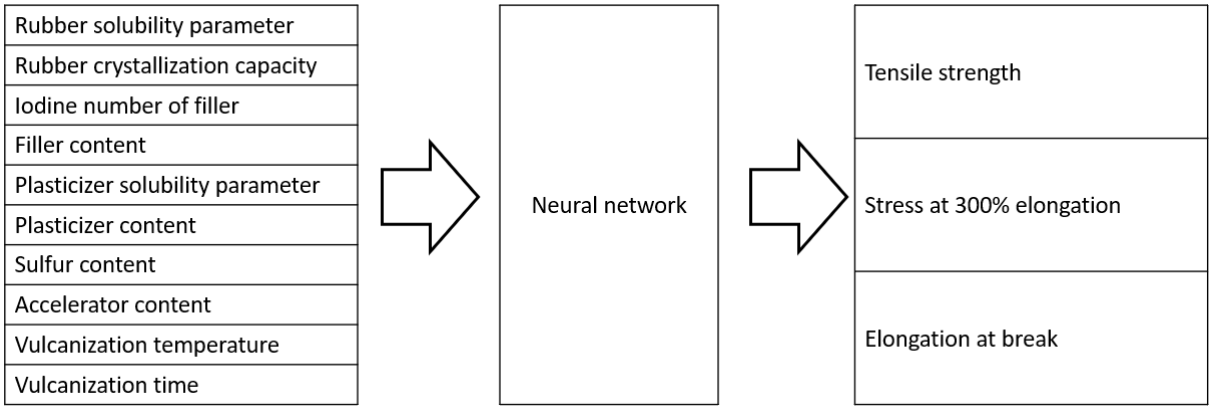


Fig. 1. Computer modeling scheme

We used the augmentation method [32–35] to expand the training sample. Data augmentation methods are widely used to improve the performance of deep learning neural networks. In the process of augmentation, training examples are modified in such a way that the number of these examples is sufficient to create deep learning neural networks. In this work, a ready-made CTGAN neural network model was used. It was trained on the available data. The CTGAN model allows to specify which columns are discrete and which are continuous. The parameters that describe the type of rubber, plasticizer or filler were taken discrete. The parameters characterizing the content of the plasticizer and filler, as well as the output parameters, were taken continuous. After the generation of new data, the data generated during the augmentation were processed, namely:

1. rounding was performed. The plasticizer's and filler's content were rounded up to integers. Output values were also rounded to integer values;
2. removal of duplicates, if any;
3. checking the generated data for out of limits.

As a result, it was possible to obtain 2,564 samples.

All the data were divided at the ratio of 70-15-15: 70 % were considered the training sample of the neural network, 15 % – as the test sample and 15 % – as the validation one.

At the first stage, the possibility to use neural networks to solve the task was fundamentally assessed, and neural network optimal parameters were also selected.

While training a neural network, there is a random factor which can lead to a change in the results produced by the trained neural network during retraining. To minimize the randomness factor, each computational experiment was carried out three times, the result obtained was averaged.

At the initial stage, the neural network of the multilayer perceptron architecture was used. At this stage, we set the tasks to evaluate the fundamental possibility of using neural network modeling methods to predict the properties of elastomers based on the known composition of rubber compounds, as well as to select the neural network parameters, which, in turn, included:

– determining optimal number of neurons in layers, with default activation and learning functions;
– selecting optimal activation functions for each layer;
– selecting optimal learning functions.

As a parameter for optimizing the neural network parameters, the mean squared error was used calculated by the formula:

$$MSE = \frac{\sum_{i=0}^{n}(y_{ex}-y)^2}{n}, \quad (2)$$

where y_{ex} is the result obtained from the neural network; y is the reference result taken from the training sample; n is the number of predicted parameters.

The parameters were optimized using the default "tansig" activation functions in the input layer, "purelin" – in the hidden layer, and the "trainlm" training function – in the output layer. Neural network modeling at this stage was carried out using the MATLAB (developed by The MathWorks).

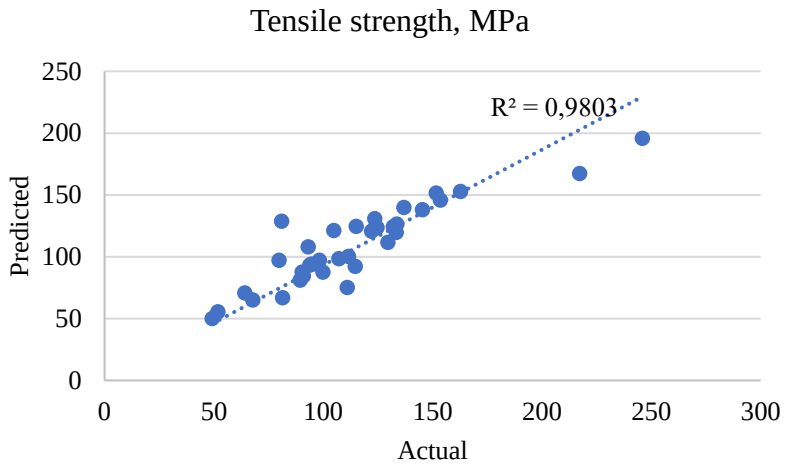
According to the results of the computational experiments, it was found that if the above activation and learning functions are used, the optimal number of neurons in the input layer is 16; in the hidden layer – 16, in the output layer – 32. With these parameters, in this series of computational experiment, the minimum value of MSE = 239.5230 was obtained for the neural network of the multilayer perceptron architecture.

Figure 2 shows the results of validating the physical and mechanical properties selected as output parameters. The trend line is drawn provided that the point intersects with the coordinates (0.0).

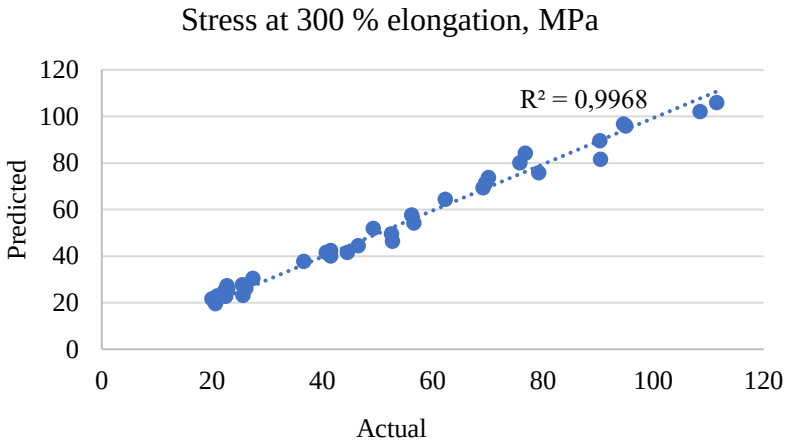
In Fig. 2, the data for two output parameters ("stress at 300 % elongation" and "elongation at break") show a high level of approximation accuracy when comparing experimentally determined and predicted neural network properties. For the output "tensile strength" parameter, the approximation accuracy is less than 0.75, which does not provide a sufficiently good level of modeling. Taking into account the fact that tensile strength is an extremely important physical and mechanical characteristic for elastomeric materials, the authors found it necessary to test neural networks of a different architecture.

In order to continue predicting operational properties of rubbers in accordance with the modeling scheme shown above (Figure 1), a program in the freely distributed Python language based on the principles of convolutional neural network architecture was developed [36]. The developed program makes it possible to perform pre-processing of the sample for training; to select the architecture of the convolutional neural network and the corresponding hyperparameters. To make selecting hyperparameters for the TensorFlow library automatic, the Keras Tuner was used. With the help of this tool, when searching for hyperparameters, we iterated:

– the ‘relu’, ‘sigmoid’, ‘tanh’, ‘elu’, ‘selu’ activation functions;
– the ‘adam’, ‘rmsprop’, ‘SGD’ learning functions;
– the number of neurons in the input layer (from 32 to 256 in increments of 16);
– the number of neurons in the hidden layer (from 32 to 256 in increments of 16).



(a)



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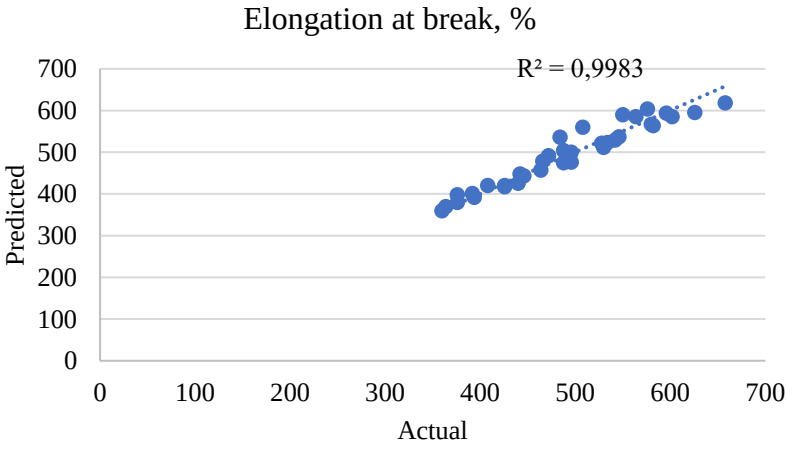


(c)

Fig. 2. Results of validating properties selected as output parameters: (a) tensile strength, MPa; (b) stress at 300 % elongation, MPa; (c) elongation at break % for the neural network of the multilayer perceptron architecture

In each case, the neural network was trained up to 8,000 epochs. As a result, it was found that the smallest error was obtained when the "relu", "elu", "selu" activation functions were used. A large prediction error was observed when the ‘sigmoid’, ‘tanh’ activation functions, as well as the "SGD" training function were used in the experiment. After a series of experiments, the "sigmoid", ‘tanh’ activation functions and the ‘SGD’ learning function were excluded from the possible iteration options.

The optimal number of iterations was determined using the validation sample. After 20,000 iterations, the error in the validation sample stopped decreasing; it even increased slightly, which proves the effectiveness of retraining. Therefore, after 20,000 iterations, the learning process was completed. To assess the quality of the neural network, cross-validation was used. The mean squared error obtained during cross-validation was 768,778.

According to the results of the computational optimization experiment, it was found that to solve the problem of predicting rubber properties, the best results should be provided by the neural network with the following parameters:

– three (input, hidden, and output) layers;
– 224 neurons in the input layer;
– 208 neurons in the hidden layer;
– 3 neurons in the output layer;
– the ‘selu’ activation function used for the input and hidden layers;
– the ‘rmsprop’ training function used;
– 20,000 iterations.

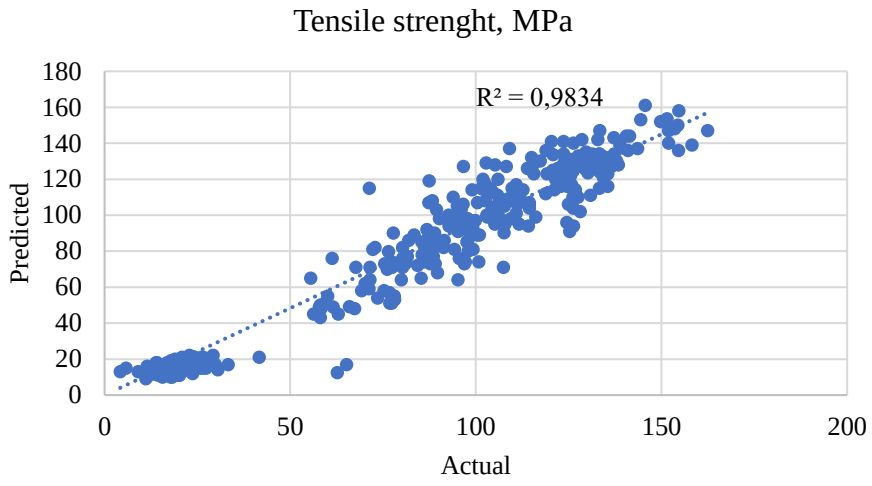
The program in the freely distributed Python language for predicting properties of rubbers using optimized hyperparameters and convolutional neural network architecture made it possible to obtain the MSE of 153.9453, against 239.5230, using the MATLAB for the neural network of the multilayer perceptron architecture, which proves the fact that the data augmentation was effective, and the neural network hyperparameters were properly selected.

Figure 3 shows the results of validating the physical and mechanical properties selected as output parameters. The trend line, as in the previous case, is drawn provided that the point intersects with the coordinates (0.0).

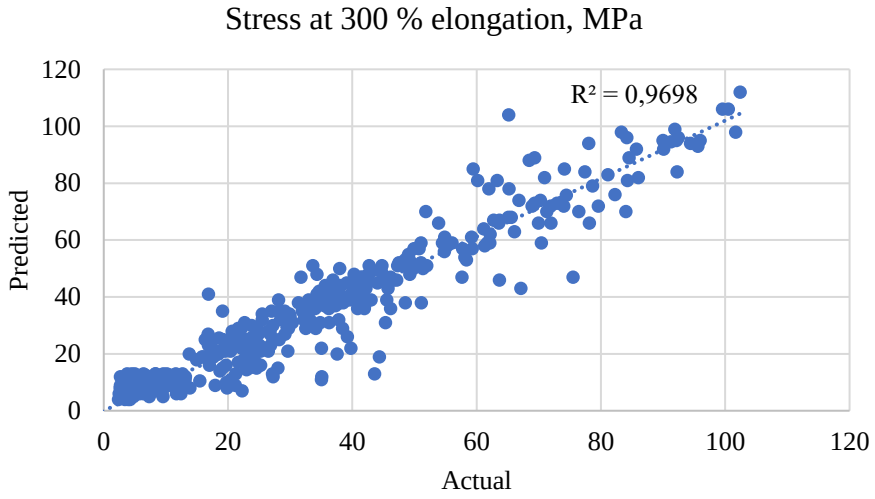
According to the presented data, a significantly higher level of approximation is obtained for the convolutional neural network architecture for the output “tensile strength” parameter. At the same time, an acceptable level of approximation is also obtained for the remaining properties, albeit slightly lower than for the neural network of the multilayer perceptron architecture. Tensile strength is predominantly considered the most important physical and mechanical property, and most other properties correlate with it. This underlines the importance of the result achieved.

Based on the results of experimental modeling, hyperparameters of the convolutional neural network were selected to predict rubber quality indicators [37].

As a result, the architecture of the convolutional neural network with two convolutional layers, three fully connected layers, and the 3×4 input matrix was chosen. At the last stage, we automatically selected the hyperparameters for the best architecture [35] which automatically selects ten characteristics of the convolutional neural network: activation functions of convolutional and fully connected layers, the number of filters in convolutional layers, the number of neurons in fully connected layers, regularization functions after each layer, the optimization function.



(a)



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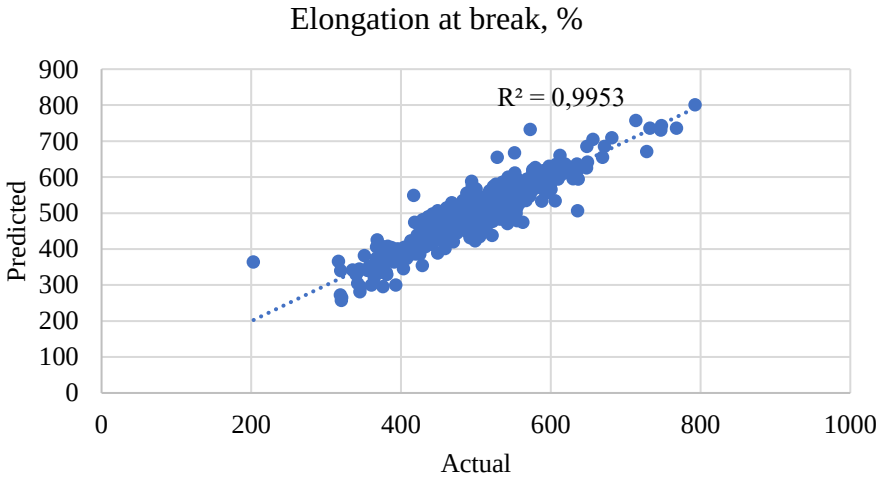

(c)

Fig. 3. Results of validating properties selected as output parameters: (a) tensile strength, MPa; (b) stress at 300% elongation, MPa; (c) elongation at break % for convolutional neural network architecture

Conclusions

Thus, based on the research results, the following conclusions can be drawn:

1. we substantiated the use of computer modeling of performance characteristics of elastomeric materials;
2. we substantiated the approaches to compiling the list of input parameters for neural network modeling, which includes the content and type of key components, as well as technological parameters of vulcanization of rubbers;
3. we proved the effectiveness of computer augmentation methods for expanding the training sample of laboratory test data. Using augmentation methods, the training sample was expanded to 2,564 samples and ensured the accuracy of experimental modeling;
4. we optimized neural network architecture and hyperparameters for modeling properties of elastomeric materials, depending on their composition and parameters of the vulcanization process;
5. we highlighted that the use of the convolutional neural network makes it possible to predict, with high accuracy, physical and mechanical properties of elastomeric materials based on butadiene, isoprene, butadiene (methyl) styrene rubbers filled with carbon black obtained during sulfur vulcanization with sulfonamide accelerators.

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