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Employment of the artificial neural networks for prediction of the mechanical properties of constructional steels

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Abstract: The paper presents employment of the artificial neural networks method for modelling the effect of the chemical composition and heat treatment parameters on the mechanical properties of the constructional steels. The method is presented for determining: yield point, tensile strength, elongation, and reduction of area.

Keywords: Neural networks, Constructional steel, Mechanical properties

1. INTRODUCTION

Constructional steels are used in building engineering and in mechanical engineering, and the most important selection criterion are their mechanical properties – most often it is their yield point. Increase of carbon concentration in carbon steels causes growth of their hardness, ultimate tensile strength and yield point, with the simultaneous deterioration of their plastic properties and ductility. The alloyed constructional steels are used for the more demanding building structures and machine elements. The main alloying elements of the constructional steels are: carbon, silicon, manganese, chromium, nickel, and molybdenum, whose main role is improving the hardenability. These steels are subjected to heat treatment to develop the martensitic structure, which makes it possible to improve their mechanical properties. Moreover, chromium, vanadium, molybdenum, and tungsten improve hardness and abrasion resistance by development of carbides.

The relationship among the technological process parameters, chemical composition, and properties feature the key information at optimisation of the manufacturing process and alloying composition for attaining the desired combination of properties for any application. Employment of statistical methods and those based on artificial intelligence, like the neural networks technology that have turned out lastly to be the very useful tool in the engineering investigation, was very helpful. The only requirement is the demand for the voluminous data needed to develop the artificial neural networks. The artificial neural networks may be employed, first of all, for prediction of properties of the existing materials, designing the new alloys, for materials selection, and optimising the manufacturing process [1-3]. Mechanical properties of materials have the key significance at their selection for any application. Basing on the artificial neural networks one can develop the computer software optimizing the chemical composition of the alloy and parameters of its heat treatment [2]. The program input parameters are the optimizing criteria, like the desired property or combination of properties.

Loops may be employed for determining the alloy's chemical composition, its heat treatment, and operating temperature. The output values are determined by the artificial neural networks and compared with all combinations of input data (chemical composition and heat treatment). The required properties are obtained as the solution, in reference to the combination of inputs.

The goal of the project was development of the artificial neural network model for determining the mechanical properties of the constructional steels, basing on their chemical compositions and heat treatment parameters.

2. MATERIALS AND METHODOLOGY

Data of about 1250 heat treated melts of the industrial constructional steels were employed in the investigations carried out. The data obtained from the steel plants include the chemical composition, heat treatment temperature, and selected mechanical properties. The detailed analysis was carried out to eliminate the corrupted data. Ranges of mass concentrations of the elements are presented in Table 1. Heat treatment of the melts included quenching and succeeding tempering. Heat treatment parameters are given in Table 2, and the mechanical properties in Table 3.

Table 1.
Ranges of mass concentrations of the analysed constructional steels elements

Range	Mass concentration of elements [wt.%]										
	C	Mn	Si	P	S	Cr	Ni	Cu	Al	Mo	V
Min	0,060	0,160	0,100	0,007	0,001	0,000	0,000	0,000	0,000	0,000	0,000
Max	0,600	1,590	0,580	0,038	0,033	14,00	2,040	0,290	1,030	1,010	0,350

Table 2.
Ranges of the heat treatment temperature values and duration times

Range	Temperature of heat treatment [^{o}C] and times [min]			
	Temperature of austenitize	Time of austenitize	Temperature of quenching	Time of quenching
Min	700	15	500	30
Max	1080	630	870	960

Table 3.
The heat treatment temperature and duration time ranges, as well as ranges of the mechanical properties of the analysed constructional steels

Range	Mechanical properties			
	R_m [MPa]	R_e [MPa]	A [%]	Z [%]
Min	218,0	442,0	12,0	26,0
Max	1130,0	1230,0	41,0	91,0

3. RESULTS

The artificial neural networks were used for development of the relationship between the steel chemical composition and its heat treatment parameters. Mass concentrations of the elements and heat treatment parameters were used as input data. Mechanical properties were presented at the network output. This set was randomly split into the training set, validation set, and the test set. The average absolute error and correlation coefficient were used to evaluate the developed model quality. Development of the network model calls for deciding the network type, the number if its hidden layers, numbers of neurons in its particular layers, activation function type, function form, variable scaling method, as well as the method and parameters of the network training. These parameters were used basing on their analysis and effect on the assumed quality coefficients. The number if neurons in the input - (15) and output layers (4) were determined. All data were subjected to linear conversion with the minimax method before entering them to the network input. Training was divided into two phases. Backpropagation algorithm was used in the first phase in 100 epochs. The second phase was carried out on 500 epochs with the conjugate gradients algorithm. The logistic functions (sigmoidal) was used as the activation function, which scaled the data in the (0;1) range. The best results were obtained for the learning rate $\eta = 0.1$ and momentum $\alpha = 0.3$. The best prediction result was obtained for the multilayer network (MLP) with the 15 – 29 – 4 structure, which means that the network has 15 input neurons (11 elements and 4 neurons referring to the heat treatment).

The values of the neural network quality coefficients for the optimum neural network model for the particular mechanical properties are given in Table 4. Figures 1-4 illustrate the comparison of the real and calculated values of the particular mechanical properties.

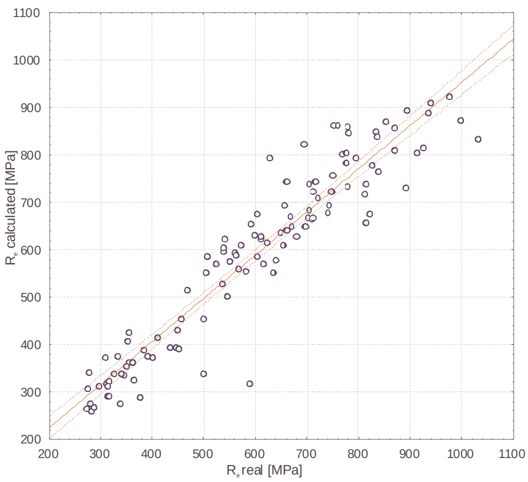

Figure 1. Real and calculated by the used of SNN value of yield point R_e

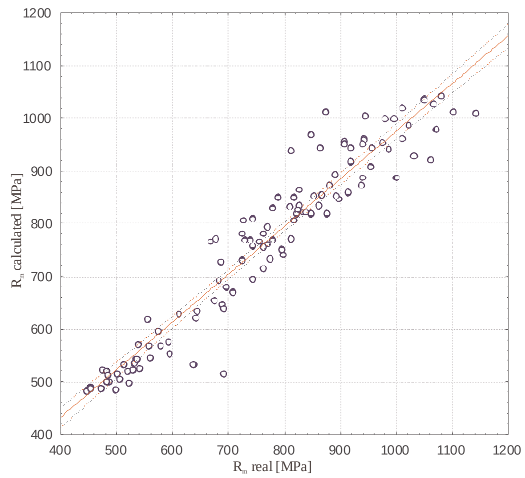

Figure 2. Real and calculated by the used of SNN value of tensile strength R_m

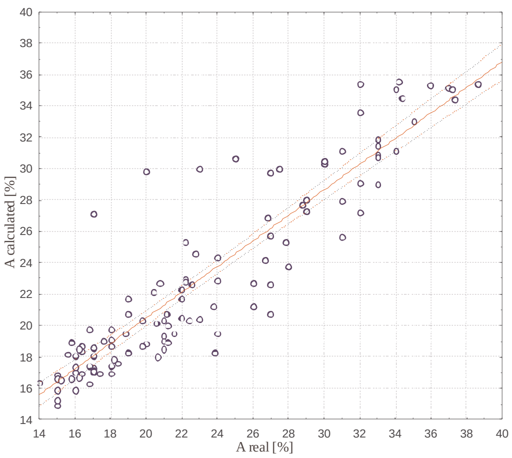

Figure 3. Real and calculated by the used of SNN value of elongation A

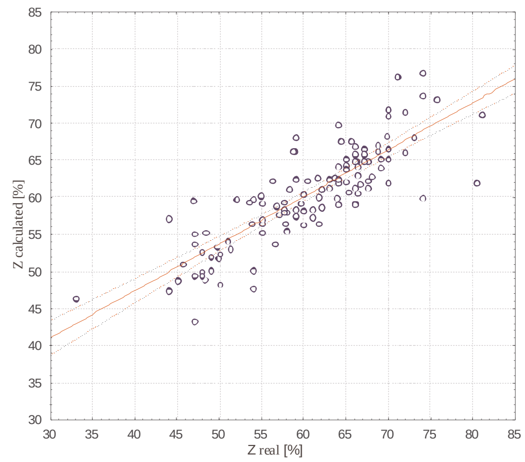

Figure 4. Real and calculated by the used of SNN value of reduction of area Z

Table 4.
Statistical values of the mechanical properties for the training-, validating-, and test sets.

Qualities	Set training	Set validating	Set testing
Yield point			
Mean [MPa]	607,2	623,9	617,7
Standard error deviation[MPa]	52,8	47,5	49,9
Pearson correlation coefficient R	0,96	0,94	0,93
Tensile strength			
Mean [MPa]	780,6	794,5	790,4
Standard error deviation [MPa]	34,8	42,3	43,8
Pearson correlation coefficient R	0,96	0,95	0,94
Elongation			
Mean [%]	22,32	21,77	21,75
Standard error deviation [%]	1,74	1,91	2,19
Pearson correlation coefficient R	0,92	0,91	0,86
Reduction of area			
Mean [%]	60,2	59,5	59,4
Standard error deviation [%]	3,4	3,8	4,1
Pearson correlation coefficient R	0,79	0,73	0,73

4. CONCLUSION

The paper presents the developed model of the artificial neural network, making modelling of the mechanical properties possible for the selected group of the constructional steels, basing on their chemical compositions and heat treatment parameters. The obtained results indicate the generalisation capability of the developed neural network.

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