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COMPUTER SIMULATION OF THE HARDENABILITY OF HEAT-TREATABLE STEELS

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ABSTRACT
The paper presents the method of modelling of the hardenability of the heat-treatable steels, basing on chemical composition. Multi-layer feedforward neural networks with learning rule based on the error backpropagation algorithm were employed for modelling of the hardenability curves. The neural networks worked out were employed for the computer simulation of the effect of particular alloying elements on the steels' hardenability. As an example of its application possibility the computer simulation was made of the influence of the particular alloying elements on hardenabiity and obtained results are presented. For the analyses the model chemical compositions of the heat-treatable steel and carburizing one were assumed. Hardness at a fixed criterial distances from the specimen end-quench test was assumed as hardenability measure.

Keywords: heat-treatable steels, computer simulation, neural network

1. INTRODUCTION

Hardenability assessment, being one of the main criteria for the selection of steel for constructional elements, makes it possible to accomplish the expected properties' distribution in the element transverse section. Hardenability depends mainly on the chemical composition. Therefore, frequent attempts to employ the numerical methods of evaluating of the steel hardenability, alternative to the experimental ones, were made. The methods known form the literature were reviewed and compared [1]. Employment of different calculation methods for steels with the same chemical composition often yields different hardenability estimation results. The incomplete pertinence of the mathematical model assumed, as well as errors committed in investigation of hardenability using a method of cooling from the specimen face, results often in discrepancy between the calculation results and the experimental data published in literature, standards, and steel catalogues. The authors' own works performed so far indicate to the necessity of developing a new method of Jominy curves calculation, more adequate to the curves obtained experimentally than the models published so far.
The paper is continuation of these works [2, 3] and presents results of computer simulation of the effect of the alloying elements on hardenability of steels.

2. MATERIALS AND METHODOLOGY

Multi-layer feedforward neural networks with learning rule based on the error backpropagation algorithm were employed for modelling of the hardenability curves. For designing, learning and testing the STATISTICA Neural Networks ver 4.0 software was employed. It was assumed that heat treatment has been done in optimal conditions for particular steel. All the neural networks considered had six input nodes and fifteen output nodes. The network architecture employed was the consequence of the assumption that the steel hardenability is mainly affected by six basic elements occurring in the alloy constructional steels, i.e. carbon, silicon, manganium, chromium, nickel and molybdenum. Six nodes of the neural network input layer correspond to the concentration of the elements mentioned. Hardness on the hardenability curve is calculated at fifteen points.

More than 500 neural networks with various number of the hidden layer and number of the hidden neurones were considered. The neural networks were trained and tested basing on the set of data consisted of information concerning the chemical compositions (concentrations of the main alloying elements occurring in theses steels' groups) and results of Jominy hardenability test of more than 1000 various heats of carburizing and heat-treatable alloy structural steel grades. During the learning procedure the number of iterations was changed in the range from 100 to 10000 and the learning coefficient in the range from 0.01 to 0.1.

For the evaluations of the neural networks considered the error E of the calculations was employed (Eq. 1):

$$E = \frac{\sum_{i=1}^{15} |M_i - C_i|}{15} \tag{1}$$

where: M_i – hardness measured at a distance i from the face, C_i – hardness calculated for a distance i from the face, i=1..15 – hardness on the hardenability curve is calculated at fifteen points (from 1,5 to 50 mm)

The verifying calculations were made for 227 heats of carburizing and heat-treatable alloy constructional steels. Value of the error E evaluating the calculation method adequacy was recorded during the procedure for each heat analysed.

As the result of the error analysis the 3 neural networks with the architecture 6-5-8-15, 6-7-7-15 with the error of calculation of 1,64 HRC, and the 6-8-8-15 with the error of 1,63 HRC were accepted. The neural networks worked out were employed for the computer simulation of the effect of particular alloying elements on the steels' hardenability. For the analyses the model chemical compositions of the steels were assumed (Tables I-IV). Hardness at a fixed criterial distance $\boldsymbol{l}$ from the specimen end-quench test was assumed as hardenability measure. As an example, the distances of 11, 25 and 40 mm were assumed.

Figures 1-4 presents the methodology of the computer simulation of the particular alloying elements effect on steel hardenability. First the hardenability curves are calculated for the particular chemical composition using the 3 neural networks worked out (designed 5_8, 7_7 and 8_8) – figure 1. Next the "average" hardenability curve is calculated (figure 2). This procedure is repeated for all chemical composition x.1-x.5 presented in tables 1-4, where x is number of variant for constant concentration of the not analysed alloying elements. The results of calculations are 5 Jominy curves for particular chemical composition of the model steels, with different concentration of the analysed alloying element – figure 3. Finally the growth of the hardness at the analysed distance from the specimen end-quench test as the effect of the analysed alloying element can be calculated (figure 4).

Table I: Chemical composition of the model steels for the analysis of the chromium effect

Steel	Mass concentration of the alloying element, %					
	C	Mn	Si	Cr	Ni	Mo
1.1	0.36	0.7	0.3	**0.5**	0.2	0.05
1.2	0.36	0.7	0.3	**0.75**	0.2	0.05
1.3	0.36	0.7	0.3	**1**	0.2	0.05
1.4	0.36	0.7	0.3	**1.25**	0.2	0.05
1.5	0.36	0.7	0.3	**1.5**	0.2	0.05
2.1	0.36	0.7	0.3	**0.5**	0.2	0.15
2.2	0.36	0.7	0.3	**0.75**	0.2	0.15
2.3	0.36	0.7	0.3	**1**	0.2	0.15
2.4	0.36	0.7	0.3	**1.25**	0.2	0.15
2.5	0.36	0.7	0.3	**1.5**	0.2	0.15
3.1	0.36	0.7	0.3	**0.5**	1	0.15
3.2	0.36	0.7	0.3	**0.75**	1	0.15
3.3	0.36	0.7	0.3	**1**	1	0.15
3.4	0.36	0.7	0.3	**1.25**	1	0.15
3.5	0.36	0.7	0.3	**1.5**	1	0.15

Table II: Chemical composition of the model steels for the analysis of the manganium effect

Steel	Mass concentration of the alloying element, %					
	C	Mn	Si	Cr	Ni	Mo
4.1	0.36	**0.5**	0.3	0.8	0.2	0.05
4.2	0.36	**0.7**	0.3	0.8	0.2	0.05
4.3	0.36	**0.9**	0.3	0.8	0.2	0.05
4.4	0.36	**1.1**	0.3	0.8	0.2	0.05
4.5	0.36	**1.3**	0.3	0.8	0.2	0.05
5.1	0.36	**0.5**	0.3	1.1	0.2	0.05
5.2	0.36	**0.7**	0.3	1.1	0.2	0.05
5.3	0.36	**0.9**	0.3	1.1	0.2	0.05
5.4	0.36	**1.1**	0.3	1.1	0.2	0.05
5.5	0.36	**1.3**	0.3	1.1	0.2	0.05
6.1	0.36	**0.5**	0.3	0.8	0.2	0.15
6.2	0.36	**0.7**	0.3	0.8	0.2	0.15
6.3	0.36	**0.9**	0.3	0.8	0.2	0.15
6.4	0.36	**1.1**	0.3	0.8	0.2	0.15
6.5	0.36	**1.3**	0.3	0.8	0.2	0.15

Table III: Chemical composition of the model steels for the analysis of the nickel effect

Steel	Mass concentration of the alloying element, %					
	C	Mn	Si	Cr	Ni	Mo
7.1	0.36	0.7	0.3	0.9	**0.2**	0.05
7.2	0.36	0.7	0.3	0.9	**0.5**	0.05
7.3	0.36	0.7	0.3	0.9	**0.8**	0.05
7.4	0.36	0.7	0.3	0.9	**1.1**	0.05
7.5	0.36	0.7	0.3	0.9	**1.5**	0.05

Table IV: Chemical composition of the model steels for the analysis of the molybdenum effect

Steel	Mass concentration of the alloying element, %					
	C	Mn	Si	Cr	Ni	Mo
8.1	0.36	0.7	0.3	0.9	0.2	**0.02**
8.2	0.36	0.7	0.3	0.9	0.2	**0.09**
8.3	0.36	0.7	0.3	0.9	0.2	**0.16**
8.4	0.36	0.7	0.3	0.9	0.2	**0.23**
8.5	0.36	0.7	0.3	0.9	0.2	**0.3**

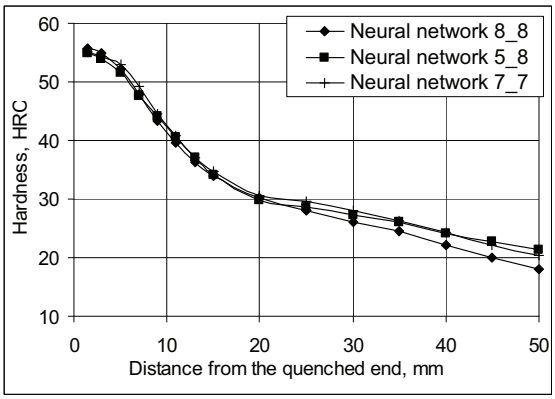

Figure 1: Calculated hardenability curves for the steel with chemical composition no 1.2.

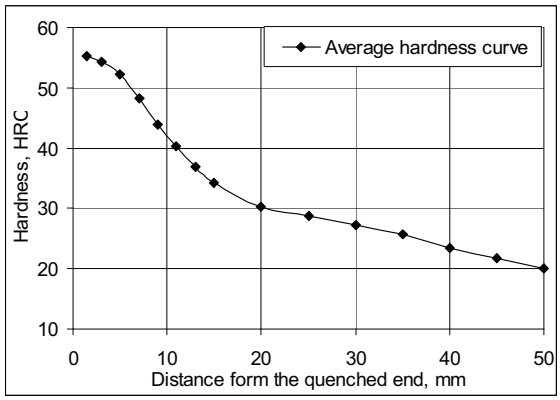

Figure 2: Average hardenability curves for the steel with chemical composition no 1.2.

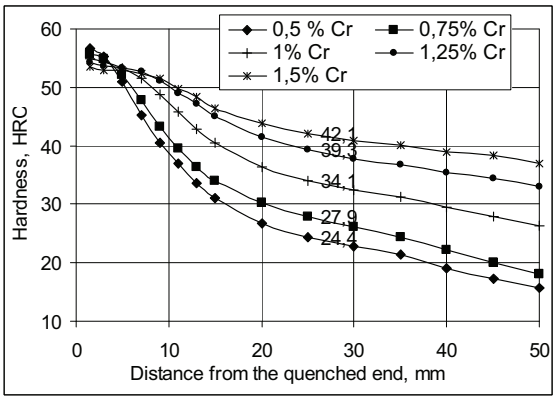

Figure 3: Calculated hardenability curves for the steels with chemical compositions no 1.1 – 1.5

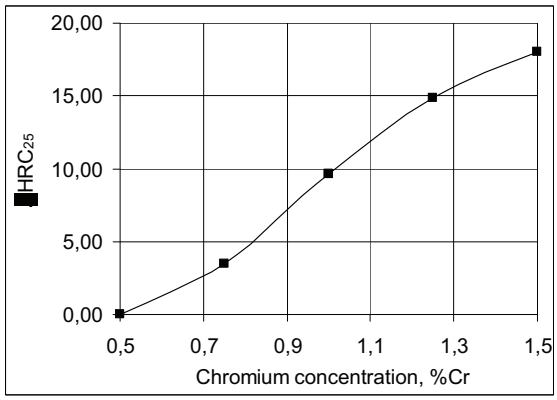

Figure 4: The effect of the Cr concentration on hardness H_{25} for the 25 mm distance from the Jominy specimen end-quench test

3. COMPUTER SIMULATION OF THE EFFECT OF ALLOYING ELEMENTS ON HARDENABILITY OF HEAT-TREATABLE STEELS

Described calculation procedure was employed for the model steels with chemical compositions presented in tables 1-4. There were analysed 4 alloying elements: chromium, manganium, nickel and molybdenum. In the case of Cr and Mn the effect on the hardenability presents fig 5 and 6 according to chemical compositions presented in tables 1 and 2. The effect of Ni and Mo presents figures 7 and 8 according to chemical compositions presented in tables 3 and 4.

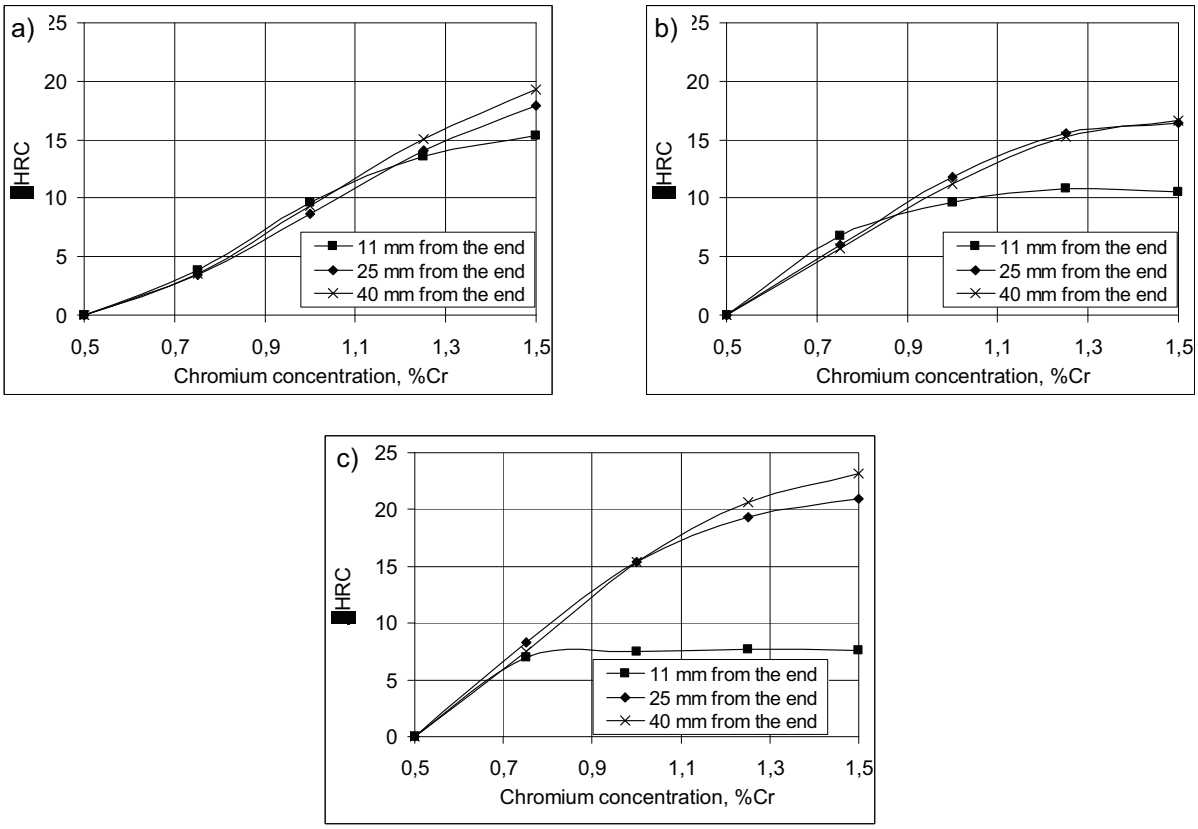

Figure 5: The effect of Cr concentration on hardenability (a - chemical compositions no 1.x, b- chemical compositions no 2.x, c- chemical compositions no 3.x – Table I)

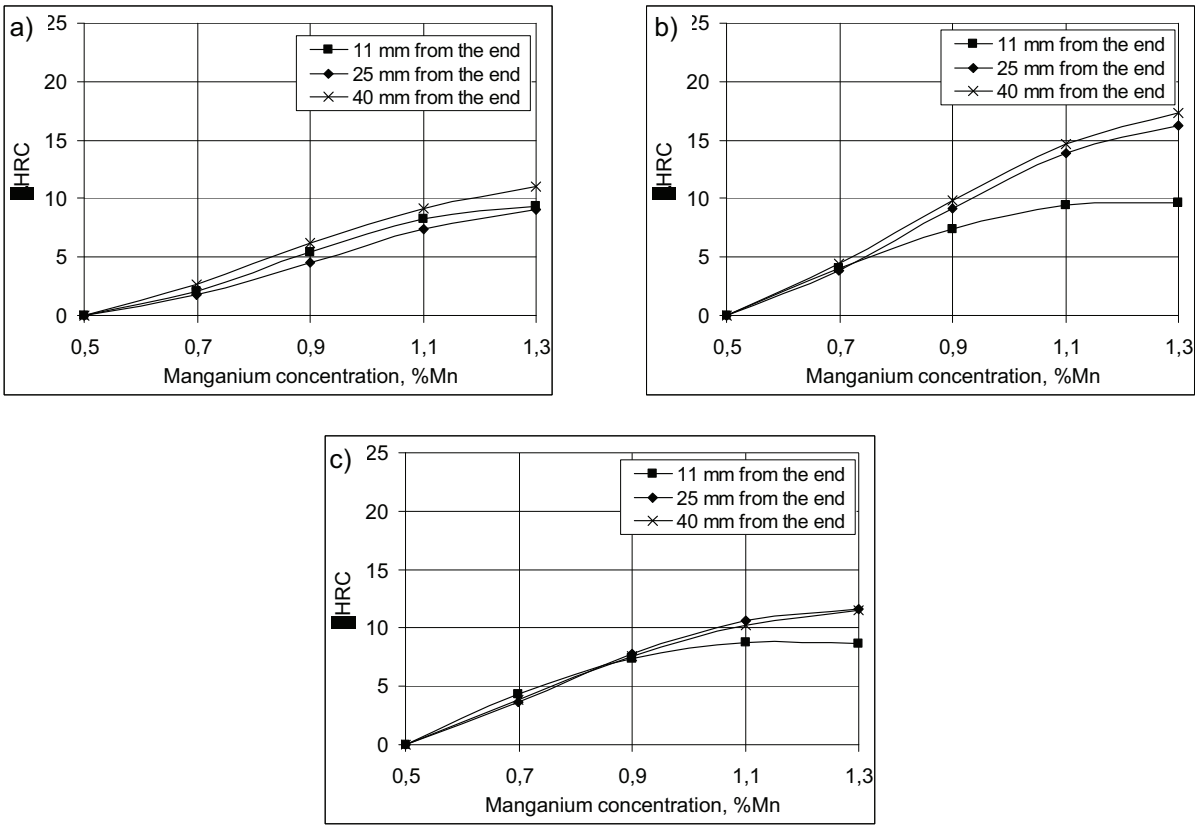

Figure 6: The effect of Mn concentration on hardenability (a - chemical compositions no 4.x, b- chemical compositions no 5.x, c- chemical compositions no 6.x – Table II)

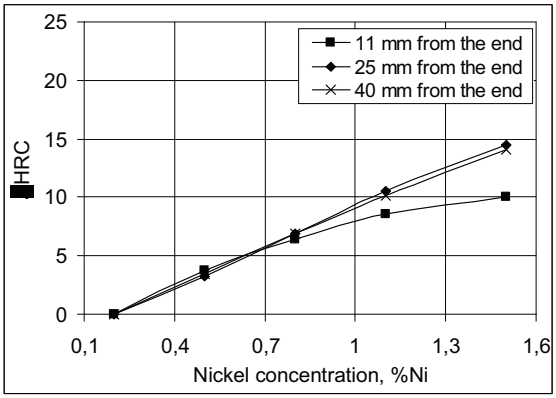

Figure 7: The effect of Ni concentration on hardenability for the chemical compositions no 7.x (Table III)

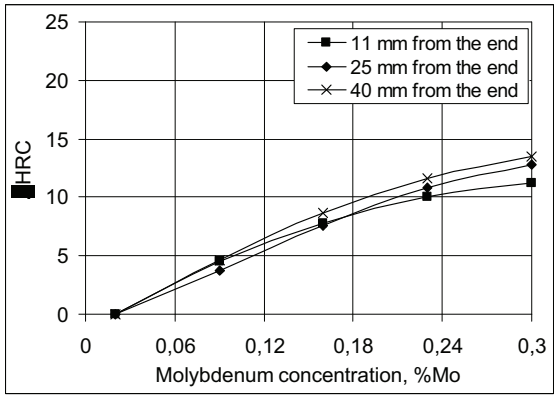

Figure 8: The effect of Mo concentration on hardenability for the chemical compositions no 8.x (Table IV)

It is possible to work out the plots presenting the effect of the concentration of an element on hardness of the analysed steel at a freely chosen distance from the Jominy specimen face. As an example of such plots, figures 5-8 presents the effect of selected elements on hardenability hardness at the distances of 11, 25 and 40 mm from the specimen face. Constant concentrations of the other elements were assumed as it is included in tables 1-4. Comparison of the data from figures 5-8 with the results of classical works by M.A. Grossman [4], I.R.

Kramer, S. Siegel and J.G. Brooks [5] and by A.F. De Retana and D.V. Doane [6] proves that the conclusions concerning the subject, presented in the works mentioned, are right. The classical investigations' results do not provide evaluation of the effect of two or more alloying elements on hardenability. One can think that this is one of the main reasons for deficiency of the existing methods of evaluation of the effect of the elements on hardenability. The example presented, however, makes it possible to determine which combinations of the alloying elements considerably increase hardenability of steel.

4. FINAL REMARKS

The paper presented application of method of hardenability modelling for evaluation of the effect of the alloying elements on steels' hardenability, using neural networks. Vast potential use of the computer tools developed was pointed out, and their practical usefulness was illustrated by examples. The developed neural network model can also be employed for simulations of the relationship between hardness at a given distance from the Jominy specimen face and the chemical composition of steel. This can be done in the entire range of concentrations of the main alloying elements occurring in constructional alloy steels. Application of the presented method, using the computer program developed, enables a scientist to make free analyses of the effect of the alloying elements occurring in heat-treatable alloy constructional steels using only computer simulation, without having to carry out additional and expensive experimental investigations.

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