EFFECTS OF ALLOYING ELEMENTS CONCENTRATION AND COOLING RATE ON CONTINUOUS COOLING TRANSFORMATIONS PREDICTED BY NEURAL NETWORK

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Abstract. The paper presents the methodology of modelling using the neural networks of the relationship between the chemical composition and austenitising temperature, and the supercooled austenite transformation kinetics during the continuous cooling. The model worked out makes it possible to calculate a complete CCT diagram for the steel with a known chemical composition and analysis of the influence of particular elements on the characteristic points and transformation curves of the supercooled austenite, and also the hardness resulting from cooling. It makes also possible forecasting of the structure developed in steel as a result of cooling at a particular rate, by the quantitative description of the percentages of ferrite, pearlite, bainite, and martensite with the retained austenite. Significant application potential of the method worked out has been demonstrated for forecasting the CCT diagrams for the newly developed steels, simulation of the alloying elements' effect, austenitising temperature and cooling rate on the shape of the supercooled austenite transformation curves, structure and hardness of steels cooled from the austenitising temperature.

Keywords. *Neural networks, CCT diagrams, Modelling.*

1. Introduction

The appropriate selection or design of a material meeting the assumed requirements features an essential stage in the contemporary design process of machines and their elements. The extensive set of the available materials and the need for the multi-criteria optimization of their selection causes employment of the computer aided material selection becoming a necessity, especially in the presence of the growing demands that the contemporary products have to satisfy. The computer aided materials selection system (CAMS) should have the auxiliary tools making possible, for instance such tasks as computer simulation of the chemical composition effect on the required properties or optimization of the feasible solutions basing on the assumed criteria - all these tasks are not supported by the engineering materials databases. Meeting the requirements mentioned above calls for the appropriate numerical model. Neural networks, employed more and more often also in the area of materials engineering may be used, among others, to develop such model. Growing popularity of the neural networks results from the feasibility to represent relationships between the investigated quantities with no need to know the physical model of the described phenomena. Results provided by the neural network demonstrate very often better consistence with the experimental data than results obtained using the empirical formulae or using the mathematical models of the analyzed processes [Bhadeshia, 1999]. Attempts to develop a model making it possible to evaluate the CCT curves basing on the chemical composition and austenitizing temperature for some selected steel groups had been made, among others, in [Van der Wolk et al., 1996, Vermulen W.G. et al., 1997, Wang J. et al. 1999]. A single neural network was used in all these cases. Mass fractions of elements and austenitizing temperature were used as input data, yielding temperatures of the particular transformations at the output, depending on the cooling rate. The results presented show the correct mapping by the network of some trends of transformation temperatures as functions of cooling time, however they differ significantly from the experimental results.

2. Material and experimental methodology

Literature data were used for developing a method for evaluation of the anisothermic transformation curves of the supercooled austenite, including chemical composition, autenitizing temperature, and the CCT curves of the constructional steels. The obtained curves were analysed, assuming mass fractions of the alloying elements as the criterion. Basing on the collected data it was assumed in addition that total of the mass fractions of manganese, chromium, nickel, and molybdenum does not exceed 5%. The ranges of the assumed mass fractions of elements and austenitizing temperature are included in Table 1.

Table 1. Ranges of mass fractions of elements and austenitizing temperatures for the analysed steels.

Range	Mass fractions of elements, %								Austenitizing temperature, °C
	C	Mn	Si	Cr	Ni	Mo	V	Cu	
Min	0.08	0.13	0.12	0	0	0	0	0	770
Max	0.77	2.04	1.90	2.08	3.65	1.24	0.36	0.3	1070

Calculating curves of the beginning and end of the transformations using a single neural network forces using a big number of neurons in the output layer, which – at the limited number of the available training curves and relatively big changes of the input values' ranges – does not allow do work out a representative training set. A satisfactory increase of the training set size is difficult because of the lack of literature data, whereas a significant limiting of the number of neurons in the output layer must result in a loss of the important information pertaining the flow of the supercooled austenite transformation. In case of a complex task, there is a possibility of splitting it into some less complicated ones and using separate networks for solving each of these problems. Therefore, while developing the algorithm for evaluating the CCT curves using the neural networks, the tasks were isolated, that could be solved with networks having less complicated structure, and organisation of the training set makes it possible to increase the number of examples with the number of the CCT curves remaining unchanged.

The method proposed in the project employs two applications of the neural networks: classification and regression. The CCT diagrams calculation process may be divided into two stages. In the first stage it was determined if along the analyzed cooling rate path zones occur of: ferrite, pearlite, bainite, and if the martensitic transformation occurs. The range of the cooling duration time, characteristic for the particular transformations, and types of the structure constituents occurring in the steel after cooling were determined as a result of the classification process. Further, temperature values were calculated of start and end of the particular transformations for each of the analyzed cooling rates. Information regarding the types of the structure constituents that originated in the steel as a result of its cooling at a particular rate was used to determine steel hardness and percentage portions of: ferrite, pearlite, bainite, and martensite with the retained austenite. The method consists of four modules: data entry module, classification module, calculation module, set of conditional statements. The outputs from the particular modules feature the data that unequivocally defines the form of the CCT diagram and are the basis for its graphical representation. The task of the data entry module is receiving information like chemical composition and austenitizing temperature and linking them with the cooling rates. The classification module composed of classifiers based on the neural networks carries out the task of identification of the structural elements occurring in the steel after completing its continuous cooling at a pre-determined rate. The calculation module employs neural networks for determining the critical values of the time and temperature of transformations, temperatures of beginning and end of transformations, hardness, as well as fractions of the structural elements. Some information from the classification and calculation modules is processed using rules included in the fourth module.

Division of the main task, consisting in calculation of the transformations' start and end curves into the partial tasks, limited to determining the start or end of a single transformation, assuming a certain saddled calculation error, may result in failing to satisfy the following conditions:

$$F_s > F_f \geq P_s > P_f \geq B_s > B_f \geq M_s \tag{1}$$

where:

F_s, F_f, P_s, P_f, B_s, B_f - temperatures of start and end of the following transformations: ferritic, pearlitic, bainitic;
M_s – temperature of the martensitic transformation start.

I was assumed that occurrence zones of the successive transformations do not have a common line determining an end of one transformation and start of another one, should the difference between the calculated temperatures be greater than the total of the absolute values of the Ej errors (where: j=F_s, F_f, P_s, P_f, B_s, B_f, M_s), featuring one of the quality evaluation coefficients for the developed models. Otherwise, the analyzed temperature range, enlarged with the Ej error value for the successive transformations has a common zone. Temperature T, determining simultaneously the end and start of the successive transformations was calculated using the weighted average, according to the formula:

$$T = \frac{E_1 \cdot T_2 + E_2 \cdot T_1}{E_1 + E_2} \tag{2}$$

where:

E_1, E_2 – error values for the temperature;
T_1, T_2 successive transformations.

The weighted average was also used to determine the common temperature when the condition described with formula (1) was not satisfied, which might happen for transformations characterized by a narrow temperature range at the analyzed cooling rate. Fig.1 demonstrates the method used to determine finally the temperatures of start and end of the transformation. Symbols (F_s, F_f, P_s, P_f, B_s, B_f, M_s) were used in Fig.1 to designate temperature values calculated using the neural network model; symbols (F_s^*, F_f^*, P_s^*, P_f^*, B_s^*, B_f^*, M_s^*) designate temperature values determining, along with the cooling rate, the points presented in the temperature - time coordinate system, featuring the basis for the graphical representation of the CCT diagrams. The relationship - T_1^*=śr.(T_1;T_2) is a weighted average specified by formula 2.

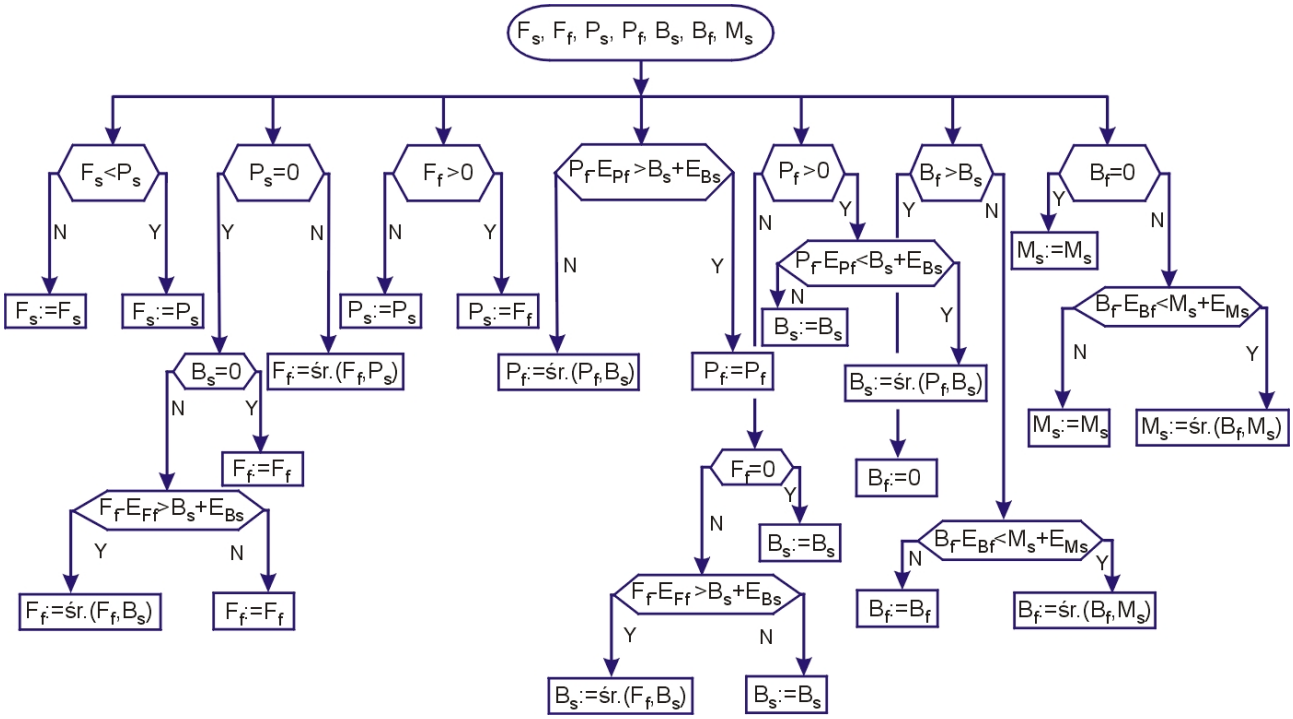

Figure 1. Algorithm for determining the temperatures of start and end of the particular transformations.

The data set used to develop the model employing the neural network was split into four subsets: training, validating, testing, and verifying one. Allocation of data to the particular subsets was done randomly. The optimum type and structure of the neural network, error function form, normalisation method for the input data, as well as training method and parameters were assumed after analysing their influence on the quality assessment coefficients of the developed models. For the regression issues the following were analysed: the average network forecast error (E_j), ratio of standard deviations of errors and data, which for the ideal forecasts assumes value of 0, as well as the Pearson's correlation coefficient r. The following quality assessment coefficients were assumed for classification problems: coefficient expressing in [%] the number of correct classifications and the area under the ROC curve. The ROC curve expresses the network sensibility (second class classified correctly) as a function of the incorrectly classified first class. In case of random classifications the area under the ROC curve assumes value of 0.5. In case of the „ideal" classifier, the area under the ROC curve assumes value of 1.

Total of 20 neural network models are used for calculating the complete CCT diagram for the assumed chemical composition using the method presented in the paper, their task is to: determine the types of the occurring transformations at given cooling rates (classification), calculate the critical temperatures of transformations (A_{c1}, A_{c3}, M_s, B_s), calculate time to start and end of the particular transformations as functions of cooling rate, calculate hardness and portions of the particular structural constituents as functions of cooling rate.

Information on neural network models used for determining the types of structural constituents occurring in the steel after the completed cooling process at a particular rate is presented in Table 2. Table 3 presents information characterizing neural networks employed for calculating the temperatures of start and end of the particular transformations as functions of the chemical compositions and cooling rate.

Table 2. Specifications of the developed classifiers based on neural networks.

Transformation area	Input parameters	Network type	Network structure	Number of cases in data sets:	Training method	Number of training epochs
Ferritic	C, Mn, Si, Cr, Ni, Mo, V, Cu, v_{ch}, T_A	MLP	10-7-1	Training - 1692	conjugate gradients	85
Pearlitic			10-15-1	Validating - 846		456
Bainitic			10-20-14-1	Testing - 846		506
Martensitic			10-12-1	Verifying - 610		1008

Table 3. Specifications of the neural networks used for calculating the temperatures of the beginning and end of the supercooled austenite transformations.

Tempe-rature	Number of cases in data sets				Input parameters	Network type	Network structure	Training method	No of epochs
	training	validating	testing	verifying					
F_s	918	459	459	327	C, Mn, Si,Cr, Ni, Mo, V, Cu, v_{ch}, T_A	MLP	10-11-1	quasi-Newton	627
F_f							10-7-1	quasi-Newton	1248
P_s	755	377	377	273			10-5-1	conjugate gradients	258
P_f							10-15-1	quasi-Newton	2124
M_s	854	427	427	319			10-11-1	conjugate gradients	84
B_s	830	415	415	284	C, Mn, Si, Cr, Ni, Mo, V, Cu, v_{ch}, T_A, B_{smaxx}		11-7-1	Lavenberg-Marquardt	430
B_f	1250	200	200	284	C, Cr, M_s, v_{ch}, B_{smax}	GRNN	5-1250-2-1	k-averages	-

3. Calculation results

In Table 4 the quality assessment coefficients of the neural networks are presented, used as classifiers yielding information on the successive transformations occurring along the analysed cooling curves. The error values, ratio of standard deviations, and the Pearson's correlation coefficient R for neural networks are given in Table 5, making it possible to determine the temperatures of beginning and end of the particular transformations as functions of cooling rate. Examples of the CCT diagrams, worked out basing on the calculations carried out, along with the experimental plots, are presented in Figures 2, 3 and 4.

Table 4. Quality assessment coefficients for neural networks, used as classifiers for determining the types of occurring transformations.

Transformation areas	Testing set		Verifying set
	Coefficient of correct classifications, %	ROC	Coefficient of correct classifications, %
Ferritic	90	0.959	91
Pearlitic	92	0.975	92
Bainitic	88	0.945	89
Martensitic	92	0.973	94

Table 5. Error values and correlation coefficients for the temperatures of beginning and end of transformations calculated for data from the testing / verifying data sets.

Tempe-rature	Error E_j, ºC	Error E_j, %	Standard deviation of the error, ºC	Ratio of standard deviations	Pearson's correlation coefficient r
F_s	18.2 / 21.6	2.6 / 3.0	18.1 / 20.3	0.52 / 0.54	0.87 / 0.85
F_f	19.4 / 20.5	3.1 / 3.2	19.2 / 17.7	0.49 / 0.50	0.87 / 0.86
P_s	15.5 / 17.1	2.4 / 2.6	14.5 / 14.8	0.54 / 0.54	0.85 / 0.84
P_f	22.8 / 21.6	3.8 / 3.6	21.3 / 18.9	0.57 / 0.55	0.80 / 0.85
B_s	25.8 / 28.4	5.3 / 5.9	27.2 / 28.0	0.58 / 0.62	0.80 / 0.79
B_f	24.1 / 26.6	7.2 / 8.0	30.9 / 32.3	0.62 / 0.64	0.78 / 0.77
M_s	21.2 / 22.4	7.1 / 8.0	19.9 / 22.2	0.53 / 0.51	0.83 / 0.86

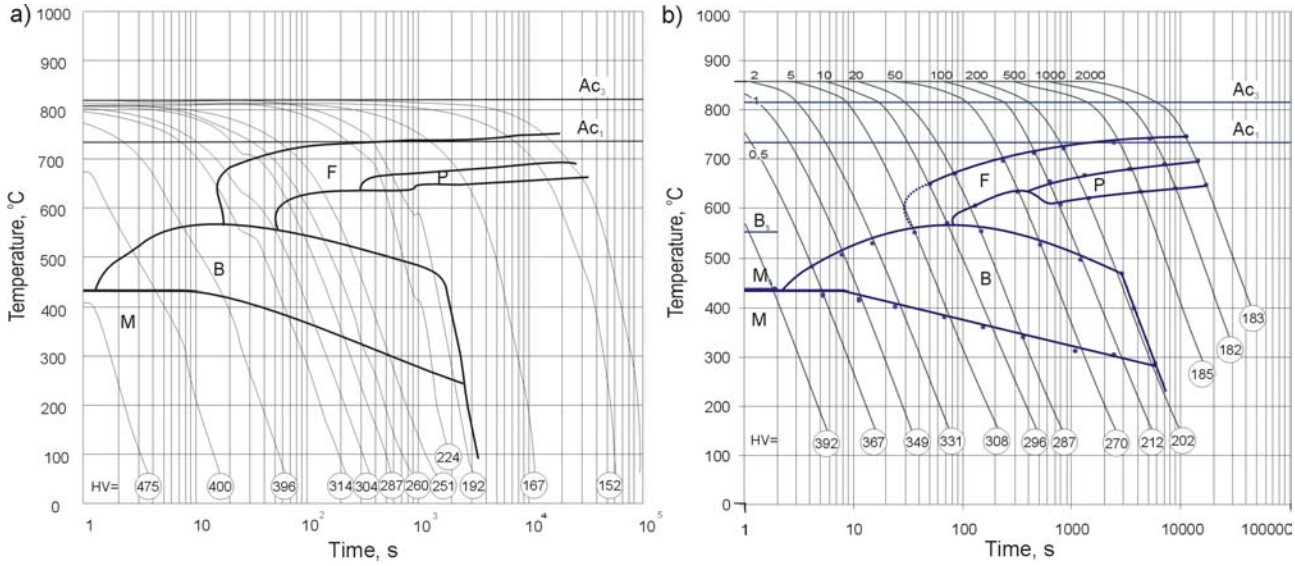

Figure 2. CCT diagram for steel with concentrations: 0.13% C, 0.51% Mn, 0.31% Si, 1.5%Cr, 1.55% Ni, 0.06% Mo, 0.01% V, austenitised at a temperature of 870ºC; a) experimental, b) calculated.

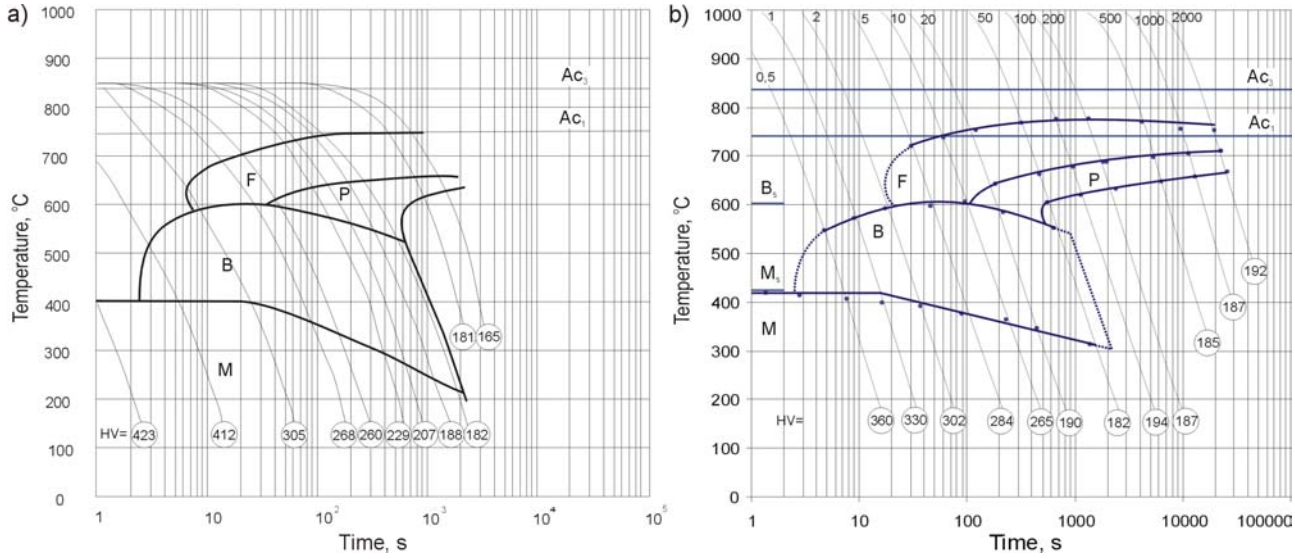

Figure 3. CCT diagram for steel with concentrations: 0.16% C, 1.12% Mn, 0.22% Si, 0.99% Cr, austenitised at a temperature of 1050ºC; a) experimental, b) calculated.

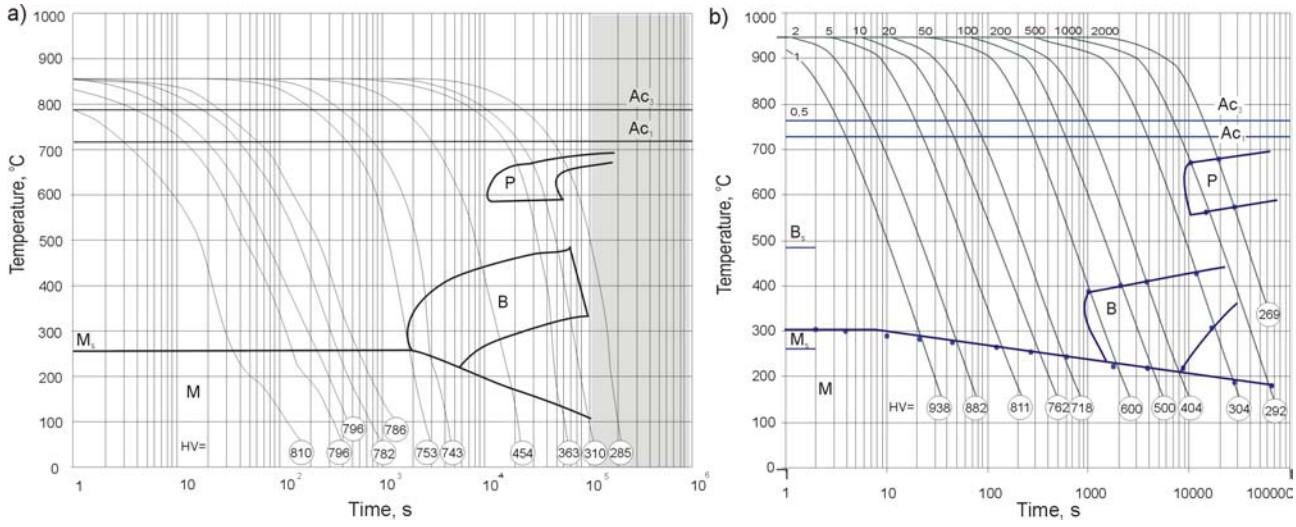

Figure 4. CCT diagram for steel with concentrations: 0.52% C. 0,52% Si, 1.09%Cr, 1.72% Ni, 0.43% Mo, 0.14% V, austenitised at a temperature of 950ºC; a) experimental, b) calculated.

4. Application example of the developed model

The synergetic effect of the alloying elements on austenite transformations during the continuous cooling is the reason for which analyzing the influence of single elements does not reveal fully their real effect. The influence of the alloying elements should be analyzed for the particular elements at the fixed concentration of the remaining constituents in the analyzed steel. The artificial intelligence tools, including the neural networks, make it possible to substitute partially the costly and time consuming experimental investigations with the computer simulation and using the obtained results as data for further analyses.

The developed neural network models make it possible to carry out computer simulation of the effect of chemical composition, austenitising temperature and/or cooling rate on a selected quantity describing austenite transformations in the CCT diagram:

- temperature of the eutectoidal transformation during heating A_{c1},
- temperature of the ferrite to austenite transformation during heating A_{c3},
- temperature of the bainitic transformation start B_s,
- temperature of the martensitic transformation start M_s,
- time referring to the lowest austenite life in the temperature range characteristic for the ferrite occurrence zone t_F,
- time referring to the lowest austenite life in the temperature range characteristic for the pearlite occurrence zone t_P,
- time to the start of the bainitic transformation, referring to the point of the shortest supercooled austenite life in the bainitic occurrence zone t_B,
- temperatures of start and end of ferrite occurrence at a particular cooling rate,
- temperatures of start and end of pearlite occurrence at a particular cooling rate,
- temperatures of start and end of bainite occurrence at a particular cooling rate,
- temperature of start of the martensitic transformation at a particular cooling rate,
- hardness of the steel cooled from the austenitising temperature at a particula rate,
- portions of ferrite, pearlite, bainite, and martensite in structure of the steel cooled from the austenitising temperature at a particular rate.

Austenitising temperature may be selected from the range presented in Table 1 or assumed basing on the A_{c3} temperature calculated using the neural network model.

The influence of a single factor, and also an arbitrary pair of factors on a selected quantity describing austenite transformations during the continuous cooling can be analysed in the steel chemical composition range presented in Table 1. The additional limitation refers to the sum of mass concentrations of manganese, chromium, nickel, and molybdenum, which should not exceed 5%. Examples of diagrams illustrating the effect of pairs of elements on the values of temperatures F_s and B_s at the fixed concentrations of other constituents are presented in Figures 5-12. One should note that analysis of the chemical composition effect on temperatures of start and end of the particular transformations calls for checking if for the assumed mass concentrations of elements, austenitising temperature, and assumed cooling rate the analysed transformation occurs. The relevant information can be obtained thanks to the developed neural classifiers.

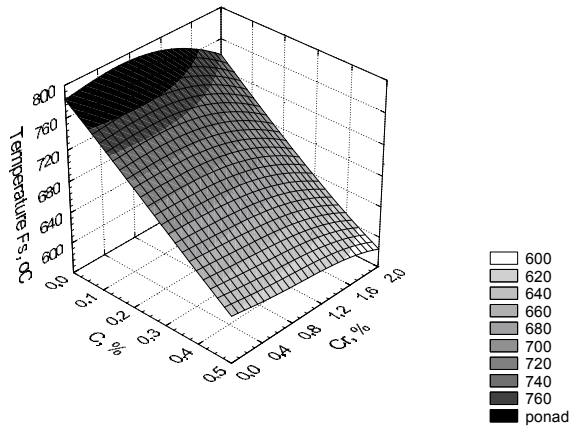

Figure 5. Effect of carbon and chromium on Fs temperature of the steel austenitised at the temperature of 1050 °C with concentrations: 1.06% Mn, 0.21% Si, 0.18% Ni, 0.02% Mo, 0.1%V; cooled at 350 °/min rate.

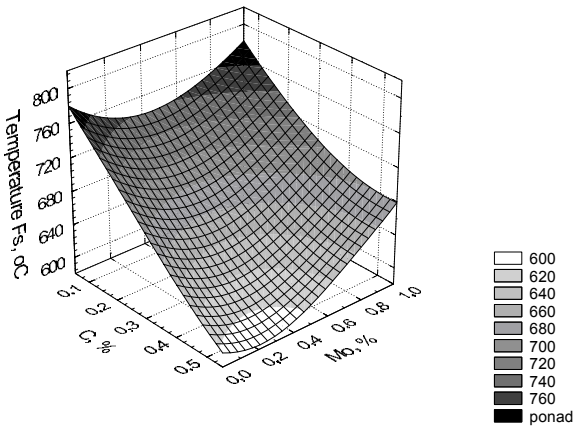

Figure 6. Effect of carbon and molybdenum on Fs temperature of the steel austenitised at the temperature of 1050 °C with concentrations: 1.06% Mn, 0.21% Si, 0.18% Ni, 0.79% Cr, 0.1%V; cooled at 350 °/min rate.

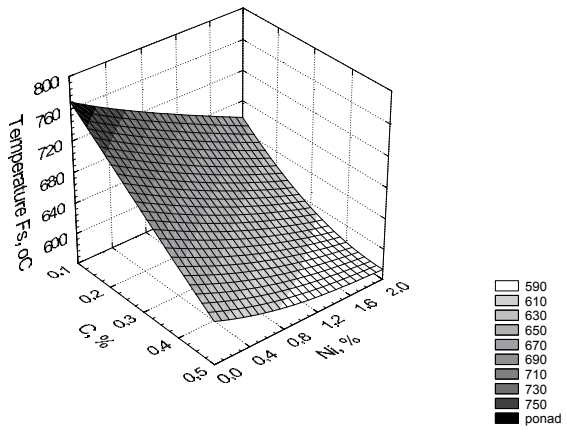

Figure 7. Effect of carbon and nickel on Fs temperature of the steel austenitised at the temperature of 1050 ^{o}C with concentrations: 1.06% Mn, 0.21% Si, 0.79% Cr, 0.02% Mo, 0.1%V; cooled at 350 ^{o}/min rate.

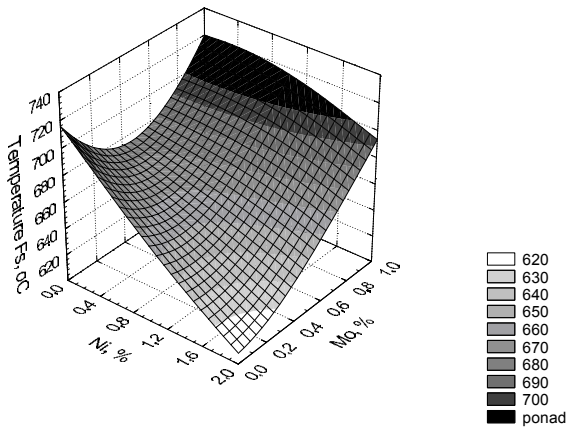

Figure 8. Effect of nickel and molybdenum on Fs temperature of th steel austenitised at the temperature of 1050 ^{o}C with concentrations: 0.24% C, 1.06% Mn, 0.21% Si, 0.79% Cr, 0.1%V; cooled at 350 ^{o}/min rate.

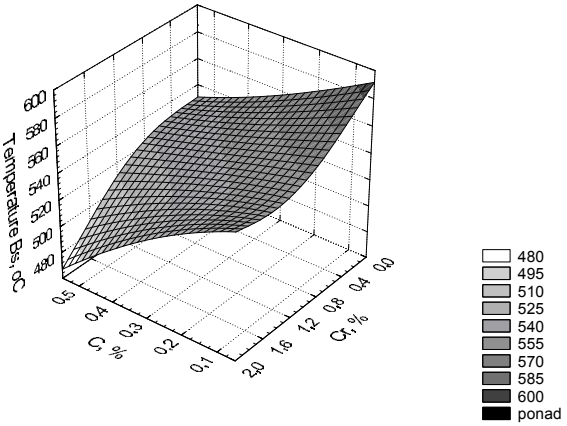

Figure 9. Effect of carbon and chromium on Bs temperature of the steel austenitised at the temperature of 850 ^{o}C with concentrations: 0.65% Mn, 0.25% Si, 0.25% Ni; cooled at 130 ^{o}/min rate.

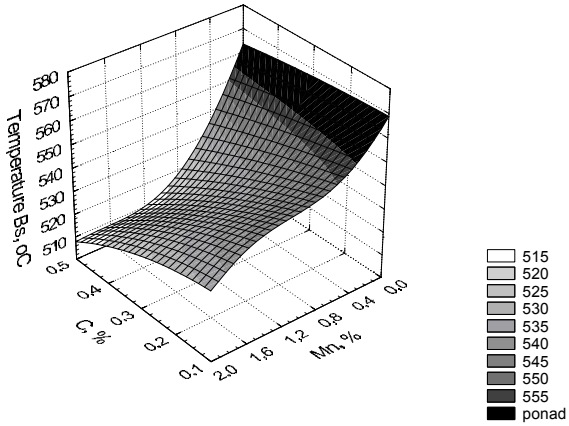

Figure 10. Effect of carbon and manganese on Bs temperature of the steel austenitised at the temperature of 850 ^{o}C with concentrations: 1.05% Cr, 0.25% Si, 0.25% Ni; cooled at 130 ^{o}/min rate.

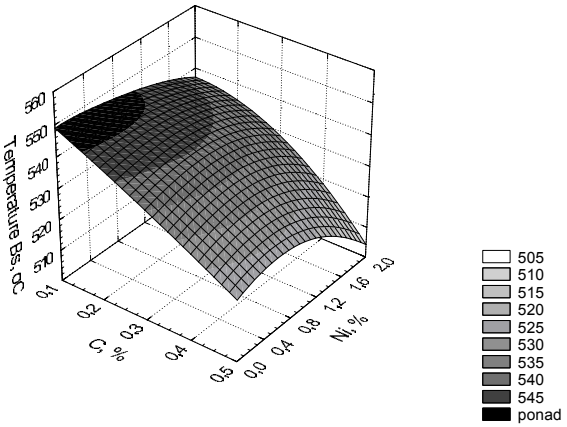

Figure 11. Effect of carbon and nickel on Bs temperature austenitised at the temperature of 850 ^{o}C with concentrations: 0.65% Mn, 0.25% Si, 1.05% Cr; cooled at 130 ^{o}/min rate.

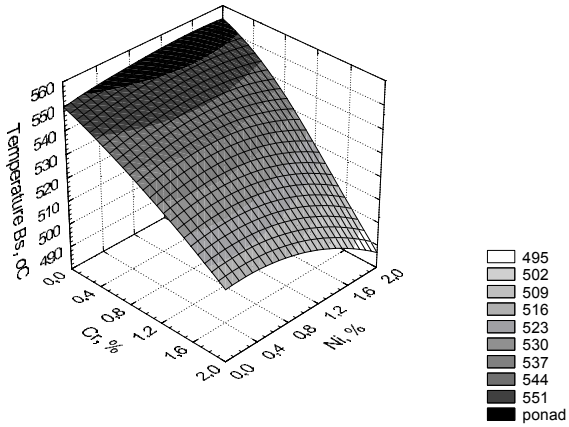

Figure 12. Effect of chromium and nickel on Bs temperature austenitised at the temperature of 850 ^{o}C with concentrations: 0.34% C, 0.65% Mn, 0.25% Si; cooled at 130 ^{o}/min rate.

4. Summary

The model developed in the project features a valuable research tool making it possible to carry out computer simulation of the effect of the chemical composition on location and shape of the supercooled austenite transformation curves or hardness obtained after cooling at the analysed rate. Using each of the models developed in this project one can determine a hypersurface originating from the values of the analysed quantity as the function of the chemical composition, austenitising temperature and/or cooling rate. Employment of the optimisation algorithms makes search possible, within the ranges of the assumed mass concentrations of the elements and values of the austenitising temperature, maximum values of the objective function on the analysed hipersurface, which leads to obtaining the optimum solution in respect to the assumed criterion. The presented procedure may be used for selection of the chemical composition of the steel and/or austenitising temperature, meeting the particular requirements connected with austenite transformations during continuous cooling, and therefore, specify the chemical composition of the steel with the predetermined CCT diagram shape. Thanks to the method developed in the project, analyses can be made referring to the effect of the selected elements on any temperature or time describing the austenite transformation and also hardness and portions of the structural constituents which originate due to cooling the steel from the austenitising temperature. One should also stress the big potential of employment of the developed model in the didactic process. The detailed description of all modules of the developed method of determining the complete CCT diagrams is presented in [Trzaska, 2002], and some of its elements in [Dobrzański et al., 2001, Dobrzański et al., 2002].

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