DOI: 10.5604/01.3001.0013.7946

Volume 97 • Issue 1 • November 2019

Journal of Achievements in Materials and Manufacturing Engineering

International Scientific Journal published monthly by the World Academy of Materials and Manufacturing Engineering

Empirical formulas for calculating Continuous Cooling Transformation diagrams

J. Trzaska

Department of Engineering Materials and Biomaterials, Silesian University of Technology, ul. Konarskiego 18a, 44-100 Gliwice, Poland

Corresponding e-mail address: jacek.trzaska@polsl.pl

ABSTRACT

Purpose: The paper presents empirical formulas for the calculation of Continuous Cooling Transformation (CCT) diagram basing on the chemical composition and austenitizing temperature.

Design/methodology/approach: In the method of calculating CCT diagrams proposed in the paper, two types of tasks are solved. First task is classification and consists in determining the range of cooling rate for particular phase transformations. The second task is regression, which aims at calculating the transformations temperature, hardness and volume fraction of phases in steel. The model of CCT diagrams was developed using multiple regression and logistic regression methods.

Research limitations/implications: CCT diagrams can be calculated according to the presented method, if the chemical composition of steel meets the criteria defined by the application range of the model.

Practical implications: The formulas presented in the article can be used to determine the conditions for heat treatment of structural steels.

Originality/value: The paper presents the method for calculating CCT diagrams of the structural steels and engineering steels, depending on their chemical composition as well as austenitizing temperature.

Keywords: Computational Materials Science, Steel, Regression analysis, CCT diagrams

Reference to this paper should be given in the following way:

J. Trzaska, Empirical formulas for calculating Continuous Cooling Transformation diagrams, Journal of Achievements in Materials and Manufacturing Engineering 97/1 (2019) 21-30.

ANALYSIS AND MODELLING

1. Introduction

Knowledge about the transformation of supercooled austenite helps, among other things, determine the conditions of heat treatment operations such as quenching, normalizing or full annealing. The Continuous Cooling Transformation (CCT) diagrams provide information on the transformations start and finish temperatures, hardness of steel and volume fractions of structural constituents for particular cooling rate. The shape of CCT diagrams depend

mainly on the starting structure of material, chemical composition of steel, and the temperature and austenitizing time [1-3].

Attempts to model transformations of supercooled austenite were and still are taken, in parallel to experimental studies. There are two areas in modelling austenite transformations. One is linked to description of the course of austenite transformations during cooling. The other one involves calculating characteristics of steel presented by CCT diagrams: temperatures of transformations, hardness, volume fraction of structural constituents. Mathematical models of austenite transformation kinetics are defined by parameters, the values of which need to be determined based on the results of experimental studies or estimated using other models. In many cases, thermo-dynamical calculations, experimentally determined CCT diagrams or models allowing to calculate the diagrams in full, or modes limited to selected characteristics provide appropriate data. Having a CCT diagram for steel with a known chemical composition and for determined austenitizing conditions is important for correct modelling of heat treatment as well as thermo-mechanical treatment [4-6]. The models proposed in the literature are characterized by various level of simplification, which translates into various level of compliance with the phenomena occurring while cooling steel. Phase transformation models are necessary for simulation of technological processes of heat treatment or thermomechanical treatment and, as a consequence, design and optimizing of industrial processes.

There are two approaches to modelling supercooled austenite transformations. One is based on theoretical considerations, including thermodynamic calculations, the theory of diffusion, the theory of nucleation and growth. The works started – among others – by Kolmogorov [7], Avrami [8], Johnson and Mehl [9], Sheil [10], Zener [11], Hillert [12], Kirkaldy [13] and Bhadeshia [14] constitute a starting point for further analysis, the results of which are broadly represented in the global literature. The values of the model's parameters are in most cases determined based on empirical data, many times using regression, and the solutions are often obtained using numerical methods [15,16].

The other approach is related to analysis of experimental data using regression methods. The multiple regression method is especially significant. Although first formulas describing temperatures of phase transformations were presented by Payson and Savage [17] and Carapella [18] more than fifty years ago, new models are still proposed and might be used for various groups of steel. Many of the empirical formulae was collected in the works [19,20]. These formulas applies to selected transformation temperatures or hardness of steel. In addition to the multiple regression method, artificial neural networks are used as well [21-24]. The development of a representative set of empirical data is a precondition for the development of an adequate model. New results of investigation for commercial steels and model alloys as well as easy access to information provide great chance in this field.

Considering the information presented above, it can be concluded that calculating CCT diagram for steel with known chemical composition and for determined austenitizing conditions is helpful not only for determining the conditions of heat treatment operations, but also for calculating the parameters of phase transformation models using various methods. The calculation of the CCT diagram is an alternative solution for dilatometric and metallographic tests, as it reduces the time needed to obtain results and reduces the costs of laboratory tests.

The results of own research connected with modelling CCT diagrams of steel using multiple regression method as well as logistic regression method were presented in the papers [25-29]. In the papers [26,29], formulas for the purpose of the calculations of the transformations temperatures of supercooled austenite were presented. The paper [27] presents results of original work related to the modelling of hardness of steel cooled continuously from the austenitizing temperature. In the papers [28], formulas for the purpose of the calculations of the volume fractions of the structural constituents were presented.

The goal of this article is to present the complete model of CCT diagrams, which was developed using multiple regression and logistic regression methods. The article also presents formulas for calculating the temperature lines of the finish of transformations: ferritic, pearlitic and bainitic. These formulas were not published in previous articles.

2. Data for calculation

The preparation of a representative empirical data set has had a basic significance for the development of the method for calculating CCT diagrams. The set of empirical data was developed on the basis of publications containing CCT diagrams for structural and engineering steels. More than 550 CCT diagrams for structural and engineering steels were taken advantage of. The dataset prepared to develop the model was divided into the training and verification sets. The verification data set contained 25 CCT diagrams. Data from this set were used for numerical verification of the model.

CCT diagrams shape depend primarily on the chemical composition of steel and the austenitizing temperature as well as austenitizing time. However, vectors including data to calculate model parameters must contain value of all variables. The information regarding the austenitizing time as well as the austenite grain size was not available on the most of the CCT diagrams. Therefore, it was necessary to simplify and reduce the number of independent variables. It was determined that the independent variables of the CCT diagrams model would be the mass fractions of the elements: C, Mn, Si, Ni, Cr, Mo, V, Cu as well as austenitizing temperature.

Statistical analysis of data was performed to determine the range of independent variable values in which the formulas of the CCT diagrams model could be used. The values of independent variables should evenly fill the domain of the approximate function. Distributions of independent variable values were examined using descriptive statistics, scatterplots and histograms made for one as well as two independent variables. It was checked whether there were outliers of variables and multi-collinearity of independent variables was analysed. Detailed information on statistical analysis of data has been presented in [20]. The range of mass fractions of the elements in which the model can be used is shown in Table 1. The additional conditions limiting the range of application of the model are presented in Table 2.

Table 1.
Range of mass fractions of elements

Range	Mass fractions of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
min	0.10	0.28	0.13	0	0	0	0	0
max	0.68	1.98	1.90	2.5	3.85	1.05	0.38	0.38

Table 2
Additional conditions limiting the range of model application

	Mass fractions of elements, %			
	Mn+Cr	Mn+Cr+Ni	Cr+Ni	Mn+Ni
max	3.6	5.6	5.3	4.5

3. Method and results

The CCT diagrams model is based on the assumption that it is necessary to solve two types of tasks for their correct calculation. First task is classification and consists in determining the range of cooling rate for particular phase transformations. The second task is regression, which aims at calculating the transformations temperature, hardness and volume fraction of phases in steel.

For the prediction of the CCT diagram of steel with a known chemical composition, formulas have been developed on the basis of which it is possible to calculate:

- Pearlite into austenite transformation start temperature during heating Ac_1,
- Ferrite into austenite transformation finish temperature during heating Ac_3,
- Maximum temperature of bainitic transformation B_{smax},
- Martensite start temperature M_{smax},
- Temperature line of start austenite into ferrite transformation F_s,
- Temperature line of finish austenite into ferrite transformation F_f,
- Temperature line of start austenite into pearlite transformation P_s,
- Temperature line of finish austenite into pearlite transformation P_f,
- Temperature line of start austenite into bainite transformation B_s,
- Temperature line of finish austenite into bainite transformation B_f,
- Temperature line of start austenite into martensite transformation M_s,
- Volume fraction of: ferrite F, pearlite P, bainite B, martensite M,
- Steel hardness, HV.

The formulas describing the influence of the chemical composition, austenitizing temperature as well as cooling rate on the transformations temperature are presented in equations (1)-(11).

$$Ac_1 = 742 - 29 \cdot C - 14 \cdot Mn + 12.5 \cdot Si + 16 \cdot Cr - 16.8 \cdot Ni - 16 \cdot Mo + 45 \cdot V + 36 \cdot Cu \quad (1)$$

$$Ac_3 = 925 - 219.4 \cdot \sqrt{C} - 7 \cdot Mn + 39 \cdot Si - 16 \cdot Ni + 13.5 \cdot Mo + 97 \cdot V \quad (2)$$

$$B_{smax} = 771 - 231{,}5 \cdot C - 68.7 \cdot Mn - 23 \cdot Si - 58.5 \cdot Cr - 30.8 \cdot Ni - 55.4 \cdot Mo - 41 \cdot V \quad (3)$$

$$M_{smax} = 541 - 401 \cdot C - 35.5 \cdot Mn - 10{,}5 \cdot Si - 14.2 \cdot Cr - 18 \cdot Ni - 17 \cdot Mo \quad (4)$$

$$F_s = 857 - 257.5 \cdot C - 68.5 \cdot Mn + 23 \cdot Si - 19.8 \cdot Cr - 37.8 \cdot Ni - 20 \cdot Mo + 33.7 \cdot V + 26.5 \cdot Cu + 0.075 \cdot T_A - 17.2 \cdot \sqrt[4]{v_c} \quad (5)$$

$$F_f = 802 - 57 \cdot C - 74.5 \cdot Mn + 22.5 \cdot Si - 9.2 \cdot Cr - 37.7 \cdot Ni - 52.5 \cdot Mo - 35 \cdot V - 18.6 \cdot \sqrt[4]{v_c} \quad (6)$$

$$P_s = 780 - 29.7 \cdot C - 65 \cdot Mn + 23.8 \cdot Si - 29.3 \cdot Ni - 26 \cdot Mo - 21 \cdot Cu - 17.4 \cdot \sqrt[4]{v_c} \quad (7)$$

$$P_f = 707 - 42{,}5 \cdot C - 65 \cdot Mn + 21 \cdot Si - 30.6 \cdot Ni - 54 \cdot Mo - 39 \cdot V + 37 \cdot Cu + 0.047 \cdot T_A - 21 \cdot \sqrt[4]{v_c} \quad (8)$$

$$B_s = 675 - 212 \cdot C - 56.8 \cdot Mn - 17 \cdot Si - 48.7 \cdot Cr - 29 \cdot Ni - 60.5 \cdot Mo - 94 \cdot V + 0.056 \cdot T_A - 1.66 \cdot \sqrt[4]{v_c} \quad (9)$$

$$B_f = 439 - 240 \cdot C - 17 \cdot Mn - 23.5 \cdot Si - 32.7 \cdot Cr - 9.4 \cdot Ni - 17.7 \cdot Mo + 5.73 \cdot \sqrt[4]{v_c} \quad (10)$$

$$M_s = 411 - 328 \cdot C - 12.7 \cdot Mn - 2.5 \cdot Cr - 8.5 \cdot Ni - 16 \cdot Mo + 34 \cdot Cu + 6.7 \cdot \sqrt[4]{v_c} \quad (11)$$

where:
C, Mn, Si, Cr, Ni, Mo, V, Cu – mass fractions of the alloying elements; %;
T_A – austenitizing temperature, °C;
v_c – cooling rate, °C/min.

Calculation of transformations temperature lines on the CCT diagram required the calculation not only of the transformation temperature value but also the determination of the cooling rate range in which this transformation occurs. To solve this problem, classifiers were included into the model. The aim of the classifiers was to determine if the analysed transformation takes place in a steel with a known chemical composition and known austenitizing temperature during cooling at the assumed rate. Four classifiers were made in which the dichotomous dependent variable (W_x) answers the question whether there is transformation under these conditions: ferritic (W_f), pearlitic (W_p), bainitic (W_b), martensitic (W_m). In this way, information was obtained regarding the type of structural constituents that are in the steel after cooling at a assumed rate. The results of classifiers calculations were used to calculate: transformations temperatures, hardness and volume fraction of structural constituents.

The dichotomous dependent variable W_x (12), describing the occurrence in the steel of the: ferrite, pearlite, bainite, martensite is equal to 0 (there is no phase in steel), if the calculated with formula (13), the value of variable S_x is not greater than a threshold value (N). The threshold value N was determined by means of minimizing the number of incorrect classifications.

$$W_X = \begin{cases} 0 \; for \; S_X \le N \\ 1 \; for \; S_X > N \end{cases} \quad (12)$$

$$S_X = \frac{\exp(K_X)}{1 + \exp(K_X)} \quad (13)$$

where:
X= f (ferrite), p (pearlite), b (bainite), m (martensite);
N=0.5 for ferritic and pearlitic as well as martensitic transformations;
N=0.4 for bainitic transformation.

where:

$$K_f = 18.4 - 15.4 \cdot C - 1.9 \cdot Mn + 0.7 \cdot Si - 2.5 \cdot Cr - 1.47 \cdot Ni - 4.8 \cdot Mo + 2.4 \cdot V + 1.4 \cdot Cu - 0.004 \cdot T_A - \sqrt[4]{v_c} \quad (14)$$

$$K_p = 12 - 1.36 \cdot C - 2.3 \cdot Mn - 2.3 \cdot Cr - 1.4 \cdot Ni - 6 \cdot Mo + 3.9 \cdot V - 0.002 \cdot T_A - 1.2 \cdot \sqrt[4]{v_c} \quad (15)$$

$$K_b = 1.3 - 3.73 \cdot C + 0.45 \cdot Mn + 0.22 \cdot Cr + 0.18 \cdot Ni + 1.9 \cdot Mo + 0.17 \cdot \sqrt[4]{v_c} - 0.57 \cdot \sqrt{(4.35 - \sqrt[4]{v_c})^2} \quad (16)$$

$$K_m = -16.48 + 4.7 \cdot C + 2.6 \cdot Mn + 0.6 \cdot Si + 2.4 \cdot Cr + 1.2 \cdot Ni + 1.9 \cdot Mo + 4.8 \cdot Cu + 0.0057 \cdot T_A + 1.12 \cdot \sqrt[4]{v_c} \quad (17)$$

The equation (18) describes the hardness of a steel cooled at a particular rate from the austenitizing temperature.

$$HV = 3.7 + 225 \cdot C + 82.5 \cdot Mn + 28 \cdot Si + 55 \cdot Cr + 28 \cdot Ni + 53.5 \cdot Mo + 147 \cdot V + 71 \cdot Cu + 0.093 \cdot T_A - 3.8 \cdot \sqrt[4]{v_c} + 67.8 \cdot C \cdot \sqrt[4]{v_c} - 42.2 \cdot W_f - 69 \cdot W_p - 32.5 \cdot W_b + 72 \cdot W_m \quad (18)$$

where: W_f, W_p, W_b, W_m – according to formulas (12)-(17).

Moreover, the hardness of steel was described using two formulas (19)-(20) which can be used for a martensitic

structure (HV_m) as well as for the ferritic-pearlitic one (HV_{f-p}). The hardness formulas for a martensitic structure, and for the ferritic-pearlitic one, may be used if adequate classification results have been obtained. If the result of the classification is not certain, it is better to use the general formula (18).

$$HV_m = 200 + 824 \cdot C + 44 \cdot Mn + 13.7 \cdot Cr + 9.2 \cdot Ni + 171 \cdot V + 78.5 \cdot Cu + 4.13 \cdot \sqrt[4]{v_c} \quad (19)$$

$$HV_{f-p} = -90 + 247 \cdot C + 45.2 \cdot Mn + 4.4 \cdot Si + 36.8 \cdot Cr + 10.8 \cdot Ni - 4 \cdot Mo + 79 \cdot V + 0.15 \cdot T_A + 13.46 \cdot \sqrt[4]{v_c} \quad (20)$$

The formulas describing the influence of the chemical composition, austenitizing temperature as well as cooling rate on the volume fractions of the microstructural constituents are presented in equations (21)-(29).

$$F(\%) = \begin{cases} 0 \; for \; W_f = 0 \\ 0 \; for \; U_f \leq 0 \\ z \cdot U_f \; for \; U_f > 0 \end{cases} \quad (21)$$

where:

$$U_f = 116 - 132.7 \cdot C - 9.5 \cdot Mn - 3 \cdot Si - 10 \cdot Cr - 5 \cdot Ni - 4 \cdot Mo - 0.021 \cdot T_A - 6.17 \cdot \sqrt[4]{v_c} + 12.2 \cdot C \cdot \sqrt[4]{v_c} + 10.2 \cdot W_f + 5.8 \cdot W_p - 9.3 \cdot W_b - 11 \cdot W_m \quad (22)$$

where:

$$z = \frac{100}{U_f + U_p + U_b + U_m} \quad (23)$$

$$P(\%) = \begin{cases} 0 \; for \; W_p = 0 \\ 0 \; for \; U_p \leq 0 \\ z \cdot U_p \; for \; U_p > 0 \end{cases} \quad (24)$$

where:

$$U_p = -5.2 + 98 \cdot C + 3 \cdot Mn + 6.5 \cdot Si + 3 \cdot Cr - 8.2 \cdot Mo + 3.72 \cdot \sqrt[4]{v_c} - 15.3 \cdot C \cdot \sqrt[4]{v_c} - 5 \cdot W_f + 25.2 \cdot W_p - 11 \cdot W_b - 18.2 \cdot W_m \quad (25)$$

$$B(\%) = \begin{cases} 0 \; for \; W_b = 0 \\ 0 \; for \; U_b \leq 0 \\ z \cdot U_b \; for \; U_b > 0 \end{cases} \quad (26)$$

where:

$$U_b = -11.5 + 25.8 \cdot C - 7.4 \cdot Mn - 7.2 \cdot Si + 4.6 \cdot Mo - 20.8 \cdot Cu + 0.03 \cdot T_A - 9.15 \cdot C \cdot \sqrt[4]{v_c} + 13 \cdot W_f - 18.4 \cdot W_p + 34.8 \cdot W_b + 6.2 \cdot W_m \quad (27)$$

$$M(\%) = \begin{cases} 0 \; for \; W_m = 0 \\ 0 \; for \; U_m \leq 0 \\ z \cdot U_m \; for \; U_m > 0 \end{cases} \quad (28)$$

where:

$$U_m = 10.2 + 2.8 \cdot C + 13.7 \cdot Mn + 4.2 \cdot Si + 7.8 \cdot Cr + 5 \cdot Ni + 8 \cdot Mo + 14.5 \cdot Cu - 0.018 \cdot T_A + 2 \cdot \sqrt[4]{v_c} + 13.7 \cdot C \cdot \sqrt[4]{v_c} - 18.2 \cdot W_f - 12 \cdot W_p - 14.3 \cdot W_b + 23.2 \cdot W_m \quad (29)$$

where: W_f, W_p, W_b, W_m – according to formulas (12-(17).

Formulas in regression tasks were evaluated based on the mean absolute error (MAE), standard deviation of mean absolute error (SDE), Pearson correlation coefficient (R) and the quotient calculated for the standard deviation of the forecast error and the standard deviation of the values of dependent variable (QSD). The quotient of standard deviations lets to relate an error made by model to the range of values of dependent variable. The best value of this statistic is equal to 0.Values of mean absolute error, standard deviation, as well as quotients of standard deviations and the Pearson correlation coefficient obtained for the formulas describing steel transformations temperatures, hardness as well as volume fraction of structural constituent are presented in Tables 3-5.

Table 3.
Error values and correlation coefficients for the temperatures of the transformations models

Transformation temperature	MAE, °C	SDE, °C	QSD	R
Ac_1	12.4	9.2	0.36	0.78
Ac_3	14.1	10.7	0.30	0.87
B_{smax}	21.2	17.2	0.31	0.87
M_{smax}	14.8	13.3	0.24	0.93
F_s	19.5	17.4	0.33	0.86
F_f	23.6	19.9	0.38	0.81
P_s	19.5	16.3	0.38	0.80
P_f	25.2	20.3	0.41	0.75
B_s	30.6	23.0	0.42	0.72
B_f	32.7	24.7	0.43	0.70
M_s	20.5	17.2	0.30	0.88

MAE – Mean absolute error; SDE – Standard deviation of the error; QSD – Quotient of standard deviations; R – correlation coefficient

Table 4.
Error values and correlation coefficients for hardness model

	MAE, HV	SDE, HV	QSD	R
HV	48.5	38.9	0.24	0.92
HV_m	30.5	25.2	0.24	0.92
$HV_{f\text{-}p}$	22.0	13.6	0.28	0.86

Table 5.
Error values and correlation coefficients for volume fraction of structural constituent model

Microstructural constituent	MAE, %	SDE, %	QSD	R
Ferrite	7.8	9.8	0.37	0.88
Pearlite	9.9	11.3	0.39	0.86
Bainite	15.8	14.2	0.44	0.76
Martensite	12.3	12.6	0.31	0.91

Formulas in classification tasks were evaluated based on the coefficient of correct classifications. The coefficient of correct classifications was calculated as the quotient of a number of correct classifications and all cases in a data set. The values of the coefficient of the correct classifications for the particular transformations are presented in Table 6.

Table 6.
The values of correct classifications coefficient

Transformation area	Coefficient of correct classifications, %
Ferritic	85.2
Pearlitic	85.9
Bainitic	72.6
Martensitic	84.3

The start and finish lines of austenite transformation temperature are calculated independently by seven formulas. It should be assumed that every calculation result is subject to an error which may lead to unfulfilled condition (30):

$$F_s > F_f \geq P_s > P_f \geq B_s \geq B_f \geq M_s \tag{30}$$

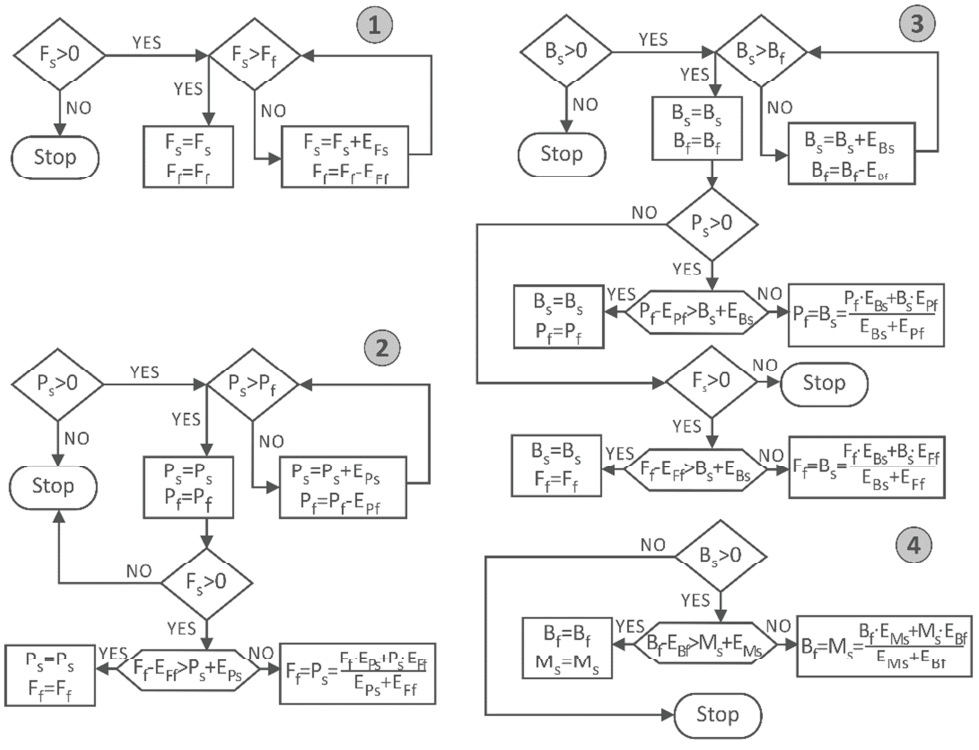

Fig. 1. Flowchart for calculating the start and the finish of the transformations temperatures

Presented on CCT diagrams, transformations of a supercooled austenite occur one by one or are separated by area of austenite. The start and the finish of the next transformation may be described by the same temperature: $F_f = P_s$, $F_f = B_s$, $P_f = B_s$, $B_f = M_s$ for the same cooling rate. Considering calculation error and condition (30), rules to determine the transformation temperatures shown in a CCT diagram were defined. The algorithm is shown in Figure 1.

The rules are executed in the order from 1 to 4. The same value will be assumed for the transformation finish and the start next transformation temperature if the absolute difference between the calculated transfomations temperatures will be lower than the sum of mean absolute errors for particular formulas. Finally, the transformation temperature was calculated as a weighted average. The mean absolute error E_i (where: i = F_s, F_f, P_s, P_f, B_s, B_f, M_s) was assumed as the weight for particular transformations. An example of calculation for a common temperature line the finish of pearlitic transformation (P_f') and the start of bainitic transformation (B_s') was presented in equation (31).

$$P_f' = B_s' = \frac{P_f \cdot E_{Bs} + B_s \cdot E_{Pf}}{E_{Bs} + E_{Pf}} \tag{31}$$

where:
P_f – according to formula (8);
B_s – according to formula (9);
E_{Pf} – mean absolute error of the equation for calculating the temperature of the finish of the pearlitic transformation;
E_{Bs} – mean absolute error of the equation for calculating the temperature of the start of the bainitic transformation.

To verify the developed model, the experimental CCT diagrams were compared with diagrams calculated using the empirical formulas. Examples of the diagrams worked out are presented in Figures 2-3. The diagrams were drawn based on the results of calculations using formulas (1)-(29). The algorithm shown in Figure 1 was also used. The CCT diagrams presented in the paper were chosen randomly from the verification data set.

It can be seen in Figures 2 and 3 that the largest errors occur in determining the range of bainitic transformation. Classifier error confirm the value of the correct classification coefficient, which is presented in Table 6. Formulas (12)-(17) make it possible to estimate whether in the microstructure of a steel cooled at a given rate from the austenitizing temperature, the following phases: ferrite, pearlite, bainite and martensite are observed. In the case of ferritic transformation and the pearlite one, the task can be reduced to looking for the highest cooling rate which is enough for the transformation to occur. Martensitic transformation requires determining the lowest cooling rate which is yet enough for the transformation to occur. Bainitic transformation needs determining two values of cooling rate limiting the field of the of it. Therefore, an additional component was introduced in formula (16) in which the current cooling rate was related with the average value of cooling rate. However, the precision of the calculations is unsatisfactory. Currently, work is underway to solve this problem.

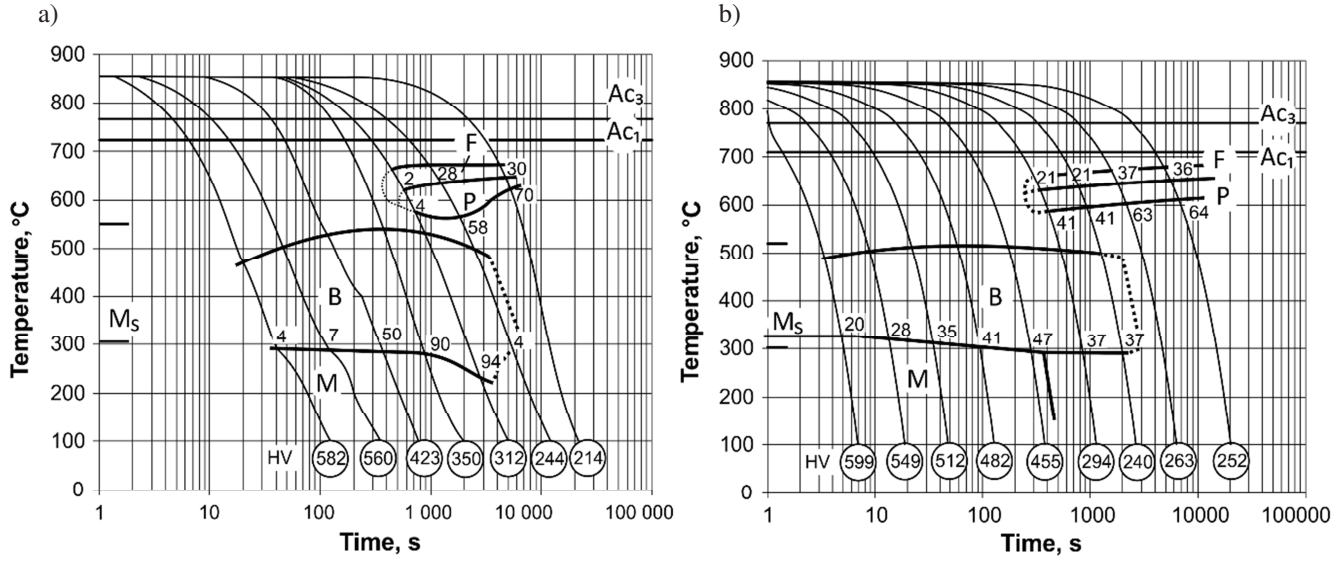

Fig. 2. CCT diagram for steel with a mass concentration of elements: 0.43%C, 0.66%Mn, 0.33%Si, 0.74%Cr, 1.4%Ni, 0.2%Mo, austenitized at temperature of 860°C; a) experimental [30], b) calculated using formulas (1)-(29)

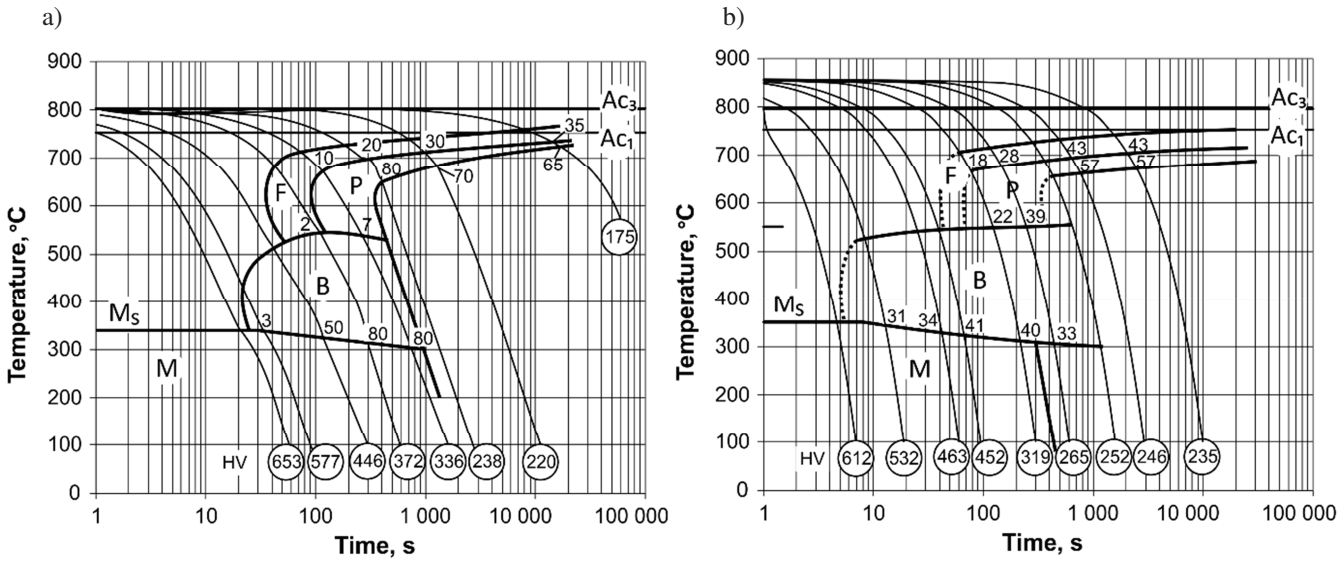

Fig. 3. CCT diagram for steel with a mass concentration of elements: 0.36%C, 0.49%Mn, 0.25%Si, 1.54%Cr, 0.21%Ni, 0.03%Mo, 0.16%Cu, austenitized at temperature of 860°C; a) experimental [31], b) calculated using formulas (1)-(29)

4. Summary

The model worked out makes it possible to calculate CCT diagram for the steel with a known chemical composition. The presented model can be used only in the range of mass fractions of alloying elements shown in the Table 1. The conditions set out in Table 2 must also be met.

Computer aided modelling is important both is industrial practice and in scientific research. It is a relatively effective and cheap method of optimizing, inter alia, conditions of technological processes, chemical composition, making it easier to obtain required properties of materials. In addition to mathematical modelling and the numerical methods related to it, biology-inspired methods are used increasingly frequently. The growing popularity of computational intelligence methods were also reflected by the area of materials engineering [32-38]. The own method of modelling the CCT diagrams with the use of neural networks has been described in detail in [20,39,40]. The neural networks model is characterized by a some smaller prediction error. For the multiple regression and logistic regression model described with the formulas (1)-(29) the mean absolute error for the temperature of transformations ranges between 12°C (Ac_1) and 33°C (temperature of the finish of bainite transformation), the mean absolute error for hardness is 48 HV and for volume fraction of structural constituents – ranges from 8% (ferrite) to 16% (bainite). The correlation coefficient values range between 0.7 and 0.93. In case of the neural model the mean absolute error for transformation temperatures ranges between 13°C (Ac_3) and 26°C (temperature of the end of bainite transformation), the mean absolute error for hardness is 33 HV, and for phase fraction – ranges from 7% (ferrite) to 12% (bainite). The correlation coefficient values range between 0.8 and 0.96.

Formulas developed using multiple regression can be easily used and distributed. This is definitely an advantage of this method. Moreover, the formulas can be easily verified by other researchers. The results of the prediction of the CCT diagrams are burdened with some errors. Those result both from simplifications using in the modelling, as well as from the character of empirical data on the basis of which the model parameters was calculated. The data set was collected based on published CCT diagrams. CCT diagrams used to calculate the parameters of the model were developed for many years in different laboratories. The error made when analysing the chemical composition, measuring the transformation temperature, hardness and volume fractions of structural constituents was undergoing important changes. A significant problem is also the graphic form of the data and errors resulting from data digitization. The accuracy of prediction of CCT diagrams can be increased if the data set is supplemented with new examples. It is particularly important to reduce classifier errors, bainite transformation temperature error and volume fraction of phases error.

Due to the limited volume of this publication only the most significant information characterizing the developed model was presented. The detailed information on the empirical data set, modelling procedure and statistics used to evaluate the model, including the statistics for the verification data set are show in the work [20].

References

[1] E. Pereloma, D.V. Edmonds (Eds.), Phase transformations in steels, Woodhead Publishing, Cambridge, 2012.

[2] J.C. Zhao, M.R. Notis, Continuous cooling transformation kinetics versus isothermal transformation kinetics of steels: a phenomenological rationalization of experimental observations, Materials Science and Engineering: R: Reports 15/4-5 (1995) 135-207, DOI: https://doi.org/10.1016/0927-796X(95)00183-2.

[3] R.C Sharma, Principles of Heat Treatment of Steels, New Age International, 2008.

[4] B. Smoljan, S. Smokvina Hanza, N. Tomašić, D. Iljkić, Computer simulation of microstructure transformation in heat treatment processes, Journal of Achievements in Materials and Manufacturing Engineering 24/1 (2007) 275-282.

[5] A. Grajcar, M. Morawiec, W. Zalecki, Austenite decomposition and precipitation behaviour of plastically deformed low-Si microalloyed steel, Metals 8/12 (2018) 1028-1039, DOI: https://doi.org/10.3390/met8121028.

[6] M. Opiela, B. Grzegorczyk, Thermo-mechanical treatment of forged products of Ti-V-B microalloyed steel, Proceedings of the Metal'2013 Conference, Brno, 2013.

[7] A.N. Kolmogorov, On statistical theory of metal crystallization, Izvestia Academy of Science USSR, ser. Math. 3 (1937) 355-360.

[8] M. Avrami, Kinetics of phase change I. General theory, Journal of Chemical Physics 7/12 (1939) 1103-1112, DOI: https://doi.org/10.1063/1.1750380.

[9] J. Johnson, R. Mehl, Reaction kinetics in processes of nucleation and growth, Transactions of the AIME 135 (1939) 416-458.

[10] E. Scheil, Anlaufzeit der austenitumwandlung, Archiv Eisenhuttenwes 8 (1935) 565-567.

[11] C. Zener, Kinetics of the decomposition of austenite, Transactions of the AIME 167 (1946) 550-583.

[12] M. Hillert, Phase equilibrium in steel, Jernkontorets Ann. 141 (1957) 757-761.

[13] J.S. Kirkaldy, B.A. Thomson, E.A. Baganis, Prediction of multicomponent equilibrium and transformation diagrams for low alloy steels, in: D.V. Doane, J.S. Kirkaldy (Eds.): Hardenability concepts with applications to steel, The Metallurgical Society of AIME, New York, 1978, 82-119.

[14] H.K.D.H. Bhadeshia, A thermodynamic analysis of isothermal transformation diagrams, Metal Science 16/3 (1982) 159-165, DOI: https://doi.org/10.1179/030634582790427217.

[15] C. Simsir, C. Hakan Gür, A FEM based framework for simulation of thermal treatments: application to steel quenching, Computational Materials Science 44/2 (2008) 588-600, DOI: https://doi.org/10.1016/j.commatsci.2008.04.021.

[16] T.C. Tszeng, G. Shi, A global optimization technique to identify overall transformation kinetics using dilatometry data-applications to austenitization of steels, Materials Science and Engineering: A 380/1-2 (2004) 123-136, DOI: https://doi.org/10.1016/j.msea.2004.03.040.

[17] P. Payson, C.H. Savage, Martensite reactions in alloy steels, Transactions ASM 33 (1944) 261-275.

[18] L.A. Carapella, Computing A or Ms (Transformation temperature on quenching) from analysis, Metal Progress 46 (1944) 108-118.

[19] A.A. Gorni, Steel forming and heat treating handbook, Available at: www.gorni.eng.br/e/Gorni_SFHTHandbook.pdf, Access in: 28.11.2019.

[20] J. Trzaska, Prediction methodology for the anisothermal phase transformation curves of the structural and engineering steels, Silesian University of Technology Press, Gliwice, 2017 (in Polish).

[21] W. Vermeulen, P.F. Morris, A.P. De Weijer, S. Van der Zwaag, Prediction of martensite start temperature using artificial neural networks, Ironmaking and Steelmaking 23/5 (1996) 433-437.

[22] W. Vermeulen, S. Van der Zwaag, P. Morris, T. De Weijer, Prediction of the Continuous Cooling Transformation diagram of some selected steels using artificial neural networks, Steel Research 68/2 (1997) 72-79, DOI: https://doi.org/10.1002/srin.199700545.

[23] J. Wang, P.J. Van Der Wolk, S. Van Der Zwaag, Effects of carbon concentration and cooling rate on continuous cooling transformations predicted by artificial neural network, ISIJ International 39/10 (1999) 1038-1046, DOI: https://doi.org/10.2355/isijinternational.39.1038.

[24] P.J. Van der Wolk, Modelling CCT-diagrams of engineering steels using neural networks, Delft University Press, Delft, 2001.

[25] J. Trzaska, L.A. Dobrzański, Modelling of CCT diagrams for engineering and constructional steels, Journal of Materials Processing Technology 192-193 (2007) 504-510, DOI: https://doi.org/10.1016/j.jmatprotec. 2007.04.099.
[26] J. Trzaska, Calculation of critical temperatures by empirical formulae, Archives of Metallurgy and Materials 61/2B (2016) 981-986, DOI: https://doi.org/10.1515/amm-2016-0167.
[27] J. Trzaska, Calculation of the steel hardness after continuous cooling, Archives of Materials Science and Engineering 61/2 (2013) 87-92.
[28] J. Trzaska, Calculation of volume fractions of microstructural components in steels cooled from the austenitizing temperature, Journal of Achievements in Materials and Manufacturing Engineering 65/1 (2014) 38-44.
[29] J. Trzaska, Empirical formulae for the calculation of austenite supercooled transformation temperatures, Archives of Metallurgy and Materials 60/1 (2015) 181-185, DOI: https://doi.org/10.1515/amm-2015-0029.
[30] Steel characteristics. Institute for Ferrous Metallurgy, Silesian Publishing House, Katowice, 1975, (in Polish).
[31] F. Wever, A. Rose, W. Strassburg, Atlas zur Warmebehandlung der Stahle, Verlag Stahleisen, Dusseldorf, 1954/1956/1958.
[32] L.A. Dobrzański, J. Trzaska, A.D. Dobrzańska-Danikiewicz, Use of neural networks and artificial intelligence tools for modeling, characterization, and forecasting in material engineering, in: S. Hashmi (Ed.), Comprehensive Materials Processing, Vol. 2: Materials Modelling and Characterization, Elsevier Science, 2014, 161-198, DOI: https://doi.org/10.1016/B978-0-08-096532-1.00215-6.
[33] S. Chakraborty, P.P. Chattopadhyay, S.K. Ghosh, S. Datta, Incorporation of prior knowledge in neural network model for continuous cooling of steel using genetic algorithm, Applied Soft Computing 58 (2017) 297-306, DOI: https://doi.org/10.1016/j.asoc.2017.05.001.
[34] N.S. Reddy, J. Krishnaiah, H.B. Young, J.S. Lee, Design of medium carbon steels by computational intelligence techniques, Computational Materials Science 101 (2015) 120-126, DOI: https://doi.org/10.1016/j.commatsci.2015.01.031.
[35] L.A. Dobrzański, T. Tański, J. Trzaska, Optimization of heat treatment conditions of magnesium cast alloys, Materials Science Forum 638-642 (2010) 1488-1493, DOI: https://doi.org/10.4028/www.scientific.net/MSF.638-642.1488.
[36] P. Papliński, W. Sitek, J. Trzaska, Modelling the structural steel hardness using genetic programming method, Advanced Materials Research 1036 (2014) 580-585, DOI: https://doi.org/10.4028/www.scientific.net/AMR. 1036.580.
[37] W. Sitek, Methodology of high-speed steels design using the artificial intelligence tools, Journal of Achievements in Materials and Manufacturing Engineering 39/2 (2010) 115-160.
[38] W. Sitek., A. Irla, The use of fuzzy systems for forecasting the hardenability of steel, Archives of Metallurgy and Materials 61/2 (2016) 797-802, DOI: https://doi.org/10.1515/amm-2016-0134.
[39] J. Trzaska, Neural networks model for prediction of the hardness of steels cooled from the austenitizing temperature, Archives of Materials Science and Engineering 82/2 (2016) 62-69, DOI: https://doi.org/10.5604/01.3001.0009.7105.
[40] J. Trzaska, A new neural networks model for calculating the continuous cooling transformation diagrams, Archives of Metallurgy and Materials 63/4 (2018) 2009-2015, DOI: https://doi.org/10.24425/amm.2018.125137.