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The calculation of CCT diagrams for engineering steels

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ABSTRACT

Purpose: of this paper is to present numerical methods for calculation of CCT diagrams for engineering steels.

Design/methodology/approach: The presented numerical methods for calculating the anisothermic diagrams of supercooled austenite are based on physical, statistical or artificial intelligence methods. In many cases input data are chemical composition and austenitising temperature. The results of calculations consist of temperature of the beginning and the end of particular transformation, the volume fraction of structural components and hardness of steel after heat treatment.

Findings: Numerical methods are an alternative to experimental measurement in providing the material data required for heat treatment process simulation.

Research limitations/implications: All presented methods for calculation of CCT diagrams for engineering steels are limited by ranges of mass concentrations of elements.

Practical implications: All presented methods may be used in computer steel selection systems for machines parts manufactured from engineering steels subjected to heat treatment.

Originality/value: The presented methods can be used for selecting steel with required structure after heat treatment.

Keywords: Computational material science; Artificial intelligence methods; Neural networks; CCT diagrams

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

The overall continuous cooling transformation kinetics can be readily described by the continuous cooling transformation (CCT) diagram. The CCT diagram is constructed by plotting a series of cooling curves onto a temperature against time diagram and then connecting the transformation start temperatures and transformation finish temperatures with separate lines. The CCT diagrams containing the quantitative data pertaining to the dependence of steel structure and hardness on temperature and time of the supercooled austenite transformations are used for determination of the structure and hardness of the quenched, normalised, or fully annealed steels. Locations and shapes of the supercooled austenite transformations' curves, plotted on the CCT diagrams, depends mostly on the chemical composition of the steel, extent of austenite homogenising, austenite grain size, as well as on austenitising temperature and time. [1]

Experimental elaboration of CCT diagram is time consuming and requires applying expensive testing equipment. It would be able to calculate CCT diagrams from the chemical composition of the steel and its austenitising temperature. Therefore, many attempts of modeling austenite transformations in the steel during cooling are being undertaken. The basis of temperature calculations and time of particular transformations of supercooled austenite and volume fraction of the particular structural components, as well as hardness obtained after cooling is finished, are most often physical models of processes proceeding in the steel during heat treatment or empirical dependences elaborated according to sufficiently big number of experimental data. The dependences allowing for modeling supercooled austenite transformations in isothermal cooling conditions, are based most often on Jonson-Mehl-Avramy[2-3] and Koistinen-Marburger [4] equations. The results of calculations obtained using mentioned equations, in many cases differ from experimental data. New relationships are published, describing various quantities connected to kinetics of supercooled austenite transformations, just for the steel with wide range of alloying elements concentration or advised for specific steel grades.

2. Neural networks model

The artificial neural networks are a universal tool for a numerical modeling capable of mapping of complex functions. The adaptation of neural networks to fulfilling a definite assignment does not require the determination of an algorithm or recording it in the form of a computer program. This process replaces learning using a series of typical stimulations and corresponding to them desirable reactions. The basic feature of neural networks is their capability to a generalization of knowledge for the new data not presented in the training process.

It was found out, basing on analysis of works [5-6], in which neural networks were employed for determining the supercooled austenite transformation curves at the continuous cooling, that development of a model making it possible to calculate the complete CCT diagrams based on a simple mapping: chemical composition and austenitising temperature → CCT diagram, must be subject to a significant forecast error. Calculating curves of the start 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 to 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 structure of the training set makes it possible to increase the number of examples with the number of the CCT curves remaining unchanged.

In papers [7-10] the own authors' method of CCT diagrams calculation has been described. 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 analysed 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 volume fraction of ferrite, pearlite, bainite, and martensite with the retained austenite. Total of 20 neural network models are used for calculating the complete CCT diagram for the assumed chemical composition and austenitising temperature. The algorithm 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.

Computer program for calculating the anisothermic diagrams of supercooled austenite is based on neural networks model. In order to design neural networks, the Statistica Neural Network, version 4.0F, software was used. [11] Representative set of data was created from the 400 of CCT diagrams, published in the literature. The range of mass concentration of elements shown in Table 1 also describes the scope of program usage.

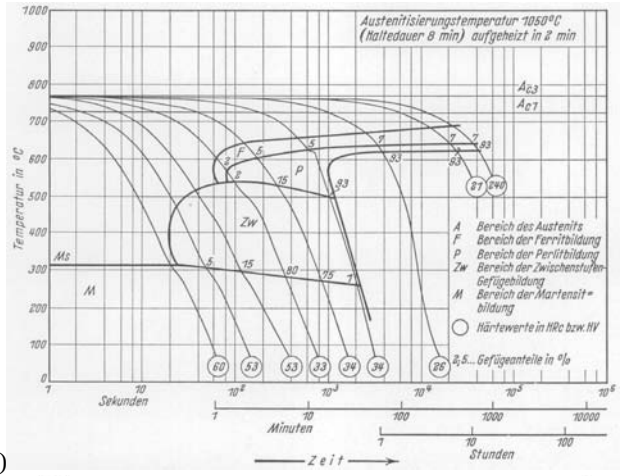
Table 1.
Ranges of mass concentration of elements

	Mass concentration of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
min.	0.08	0.13	0.12	0	0	0	0	0
max.	0.77	2.04	1.90	2.08	3.65	1.24	0.36	0.3
%Mn+%Cr+%Ni+%Mo≤5								

The program was developed in the Borland C++ Builder 6 compiler. The input data for the program were mass concentration of elements and austenitising temperature, which can be input by the user or calculated by program as temperature Ac3+50°C.
Predicted values of steel hardness and calculated volumes fractions of phases give very well results. Shapes of the CCT diagrams generated by program are very similar to experimental diagrams.

In work [5] the use of artificial neural network for the prediction of the transformation start and finish lines in Continuous Cooling Transformation diagrams was described. The data were selected from a single source [12]. In total 89 steel grades were selected for training and validation of the neural network. The input parameters of neural network were the chemical composition and the austenitising temperature. The chemical compositions was characterised using 12 alloying elements: C, Mn, Si, P, S, Cr, Ni, Mo, V, Cu, Al, N. The ranges of input parameters for the neural network are given in Table 2.

The prior austenite grain size has an important effect on the transformation kinetics, but as no information was available on this parameter for all steels, it could not be included as an input parameter. The output of the neural network was the transformation lines in the CCT diagram. The CCT diagrams had to be converted from graphical to numerical format. In this model 23 cooling curves were superimposed on each CCT diagrams and the intercepts with



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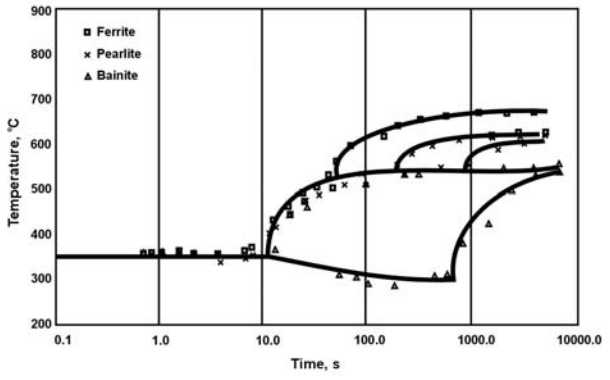

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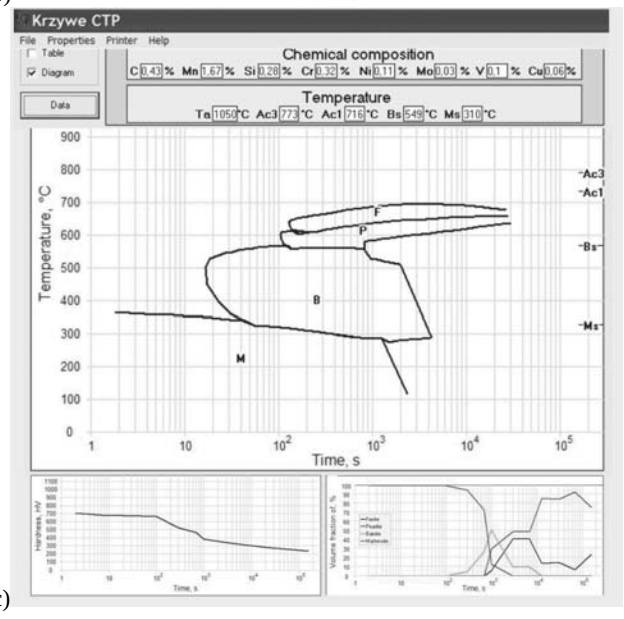


(c)

Fig. 1. CCT diagram for steel with concentrations: 0.43% C, 1.67% Mn, 0.28% Si, 0.32% Cr, 0.11% Ni, 0.03% Mo, 0.01% V, 0.06% Cu, austenitised at temperature of 1050°C: a) experimental [13], b) calculated by the neural network [5], c) calculated by the authors' method [11]

the boundary lines indicating the time temperature combination leading to a particular transformation. The number of intercepts for each cooling curves was 6. CCT diagram was determined basing on the activation level of a 138 neurons in the neural network output layer. The neural network was trained using back propagation of error learning rule and cross-validation procedure. The neural network with one hidden layer and numbers of neurons in these layers as five was assumed to be optimal.

Table 2.
Ranges of input parameter for neural network. The mass concentration of elements are expressed in % and the austenitising temperature (Ta) in °C

	Input parameter						
	C	Mn	Si	S	P	Cr	Ni
min	0.10	0.50	0	0	0	0	0
max	0.44	2.25	1.0	0.08	0.044	1.95	2.0
	Mo	V	Cu	Al	N	Ta	
min	0	0	0	0	0	850	
max	0.55	0.45	0.48	0.068	0.050	1350	

Presented results indicate to the correct representation by the network of some transformation temperature change trends versus cooling time; however, differ significantly from the experimental results. The relative standard deviation in the prediction of start and end temperatures of each transformation depended on the cooling rate. For the low and cooling rates it was ~40°C, for the intermediate it rose to 90°C for the ferrite start transformation and to 75°C for the pearlite and bainite transformations.[5] The experimental and predicted CCT diagrams are show in Figure 1 (a,b). Figure 1c presents program window with the calculated CCT diagram (authors' method).

3. The Creusot-Loire System

Research workers at the Creusot Laboratory have been studying the effect of chemical composition and austenitisation conditions on the continuous cooling transformation diagrams for carbon and low alloy steels.[14-17] They have derived the following equations:

$$\log v_M = 9.81 - (4.62 \cdot C + 1.05 \cdot Mn + 0.5 \cdot Cr + 0.66 \cdot Mo + 0.54 \cdot Ni + 0.00183 \cdot P_A) \quad (1)$$

$$\log v_{M90} = 8.76 - (4.04 \cdot C + 0.96 \cdot Mn + 0.58 \cdot Cr + 0.97 \cdot Mo + 0.49 \cdot Ni + 0.001 \cdot P_A) \quad (2)$$

$$\log v_{M50} = 8.50 - (4.13 \cdot C + 0.86 \cdot Mn + 0.41 \cdot Cr + 0.94 \cdot Mo + 0.57 \cdot Ni + 0.0012 \cdot P_A) \quad (3)$$

$$\log v_B = 10.17 - (3.8 \cdot C + 1.07 \cdot Mn + 0.57 \cdot Cr + 1.58 \cdot Mo + 0.7 \cdot Ni + 0.0032 \cdot P_A) \quad (4)$$

$$\log v_{B90} = 10.55 - (3.65 \cdot C + 1.08 \cdot Mn + 0.61 \cdot Cr + 1.49 \cdot Mo + 0.77 \cdot Ni + 0.0032 \cdot P_A) \quad (5)$$

$$\log v_{B50} = 8.74 - (2.23 \cdot C + 0.86 \cdot Mn + 0.59 \cdot Cr + 1.60 \cdot Mo + 0.56 \cdot Ni + 0.0032 \cdot P_A) \quad (6)$$

$$\log v_{FP} = 6.36 - (0.43C + 0.49 \cdot Mn + 0.26 \cdot Cr + 0.38 \cdot Mo + 2 \cdot Mo^{0.5} + 0.78 \cdot Ni + 0.0019 \cdot P_A) \quad (7)$$

$$\log v_{FP90} = 7.51 - (1.38 \cdot C + 0.35 \cdot Mn + 0.11 \cdot Cr + 2.31 \cdot Mo + 0.93 \cdot Ni + 0.0033 \cdot P_A) \quad (8)$$

where:
C, Mn, Cr, Ni, Mo, – mass concentration of the alloying elements;
v_i [°C/h] – critical cooling rates at 700°C are referred to as:
v_M-for martensite; v_{M90}- denotes 90% of martensite with 10% of other constituents; v_{M50}- denotes 50% of martensite with 50% of other constituents; v_B-for bainite; v_{B90}- denotes 90% of bainite with 10% of other constituents; v_{B50}- denotes 50% of bainite with 50% of other constituents; v_{FP}-for ferrite-pearlite; v_{FP90}- denotes 90% of ferrite-pearlite with 10% of bainite;
P_A is an austenitising parameter whose value in °C/h is given by:

$$P_A = \left[\frac{1}{T} - \frac{nR}{\Delta H} \log \frac{t}{t_o} \right]^{-1} \quad (10)$$

where:
T-temperature, K,
t – time,
t_o – unit of time,
R – gas constant 8.314 J/K·mol,
n – $\log_e 10$,
ΔH – the activation energy of the phenomenon which for grain growth in most low alloy steels has a value of 460.55 kJ/mol.

The hardness of the microstructures produced are given by the equations (11-13).

$$HV_M = 127 + 949 \cdot C + 27 \cdot Si + 11 \cdot Mn + 16 \cdot Cr + 8 \cdot Ni + 21 \cdot \log v_R \quad (11)$$

$$HV_B = -323 + 185 \cdot C + 330 \cdot Si + 153 \cdot Mn + 144 \cdot Cr + 191 \cdot Mo + 65 \cdot Ni + (\log v_R) \cdot (89 + 53 \cdot C - 55 \cdot Si - 22 \cdot Mn - 20 \cdot Cr - 33 \cdot Mo - 10 \cdot Ni) \quad (12)$$

$$HV_{F\text{-}P} = 42 + 223 \cdot C + 53 \cdot Si + 30 \cdot Mn + 7 \cdot Cr + 19 \cdot Mo + 12{,}6 \cdot Ni + (\log v_R) \cdot (10 - 19 \cdot Si + 8 \cdot Cr + 4 \cdot Ni + 130 \cdot V) \quad (13)$$

where: v_R is the cooling rate.

Maynier and coworkers have developed a useful method to predict steel hardness. Their equations were derived from 107 tests on 40 industrial grades. The total hardness of steel is calculate dependent on the volume fractions of the constituents of the microstructure.

$$HV = (\%FP \cdot HV_{F\text{-}P} + \%B \cdot HV_B + \%M \cdot HV_M)/100 \quad (14)$$

A disadvantage of the Creusot-Loire method is that knowledge is required of the amount of the starting constituents of the microstructure. This can be estimated by the equations (1-8).

A range of the accepted mass concentrations of the elements has been presented in Table 3. An example of the comparative plots showing changes of fractions of the structural constituents depending on time required to cooling the steel from the austenitising temperature are presented in Figures 2,3. Figures 4,5 presents graphical comparison of the hardness curves calculated using different methods and the experimental ones.[11,13,14].

Table 3.
Ranges of mass concentration of elements

Range	Mass concentration of elements, %						
	C	Mn	Si	Cr	Ni	Mo	V
min	0.2	0	0	0	0	0	0
max	0.5	2.0	1.0	3.0	4.0	1.0	0.2
%Mn+%Ni+%Cr+%Mo<5%							

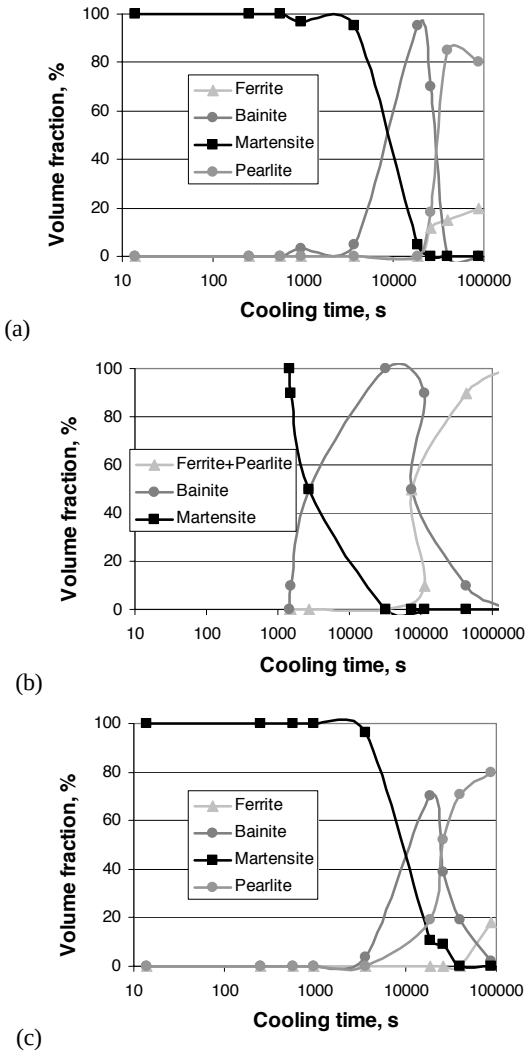


Fig. 2. Fractions of the structural constituents in steel with concentrations of : 0.46% C, 0.77% Mn, 0.23% Si, 1.13% Cr, 1.49% Ni, 0.28% Mo, 0.18% V, austenitised at 860ºC: a) experimental [13], b) calculated by the Maynier model [14], c) calculated by the authors' method [11]

4. JMatPro software

The software tool JMatPro (Java-based Materials Properties) has been developed by Thermotech and Sente Software. JMatPro is now available as a commercial product. [18]

JMatPro is a cross-platform software which calculates a wide range of materials properties and is particularly aimed at multi-components alloys used in industrial practice. These properties include TTT and CCT diagrams, physical and thermophysical properties, Jominy hardenability as well as high temperature mechanical properties. All the properties are calculated using physically based models which ensure consistent results. The

wide range of calculated properties can then be used as an input to processing simulation packages like Finite Element Modelling tools. [19].

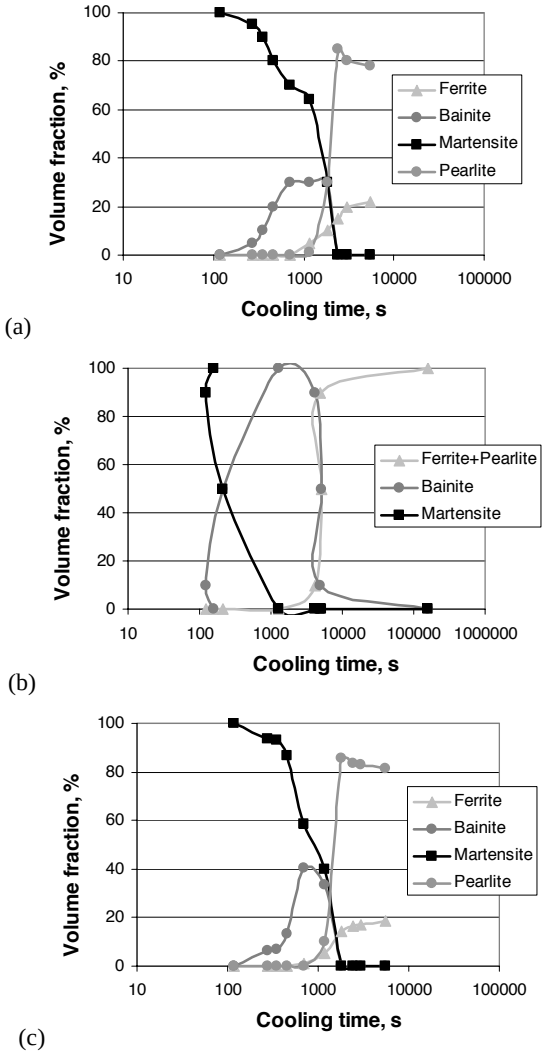


Fig. 3. Fractions of the structural constituents in steel with concentrations of : 0.43% C, 0.82% Mn, 0.41% Si, 1.22% Cr, 0.04% Ni, 0.11% V, austenitised at 880ºC: a) experimental [13], b) calculated by the Maynier model [14], c) calculated by the authors' method [11]

The user simply inputs their choice of chemical composition, austenite grain size and austenitising temperature. The thermodynamic module calculates critical temperatures (Ae3 for ferrite and Ael for pearlite). Other critical temperatures, such as the formation temperatures for bainite and martensite, are calculated from empirical formulae. Finally, the software calculates the time taken for a set amount of transformation at the desired temperatures. [19]. JMatPro based on Johnson Mehl Avrami equation [2-3]. It is possible to convert TTT diagrams to continuous-cooling-transformation diagrams using Scheil's Additivity Rule [21].

JMatPro could be used to predict TTT and CCT diagrams for general steels, including medium to high alloy types, tool steels, 13%Cr steels. [22] Maximum level of the mass concentrations of the elements has been presented in Table 4.

Table 4.
Maximum level of alloying elements in steels used for validation of the model.[19]

	Mass concentration of elements, %					
	Fe	C	Si	Mn	Ni	Cr
min.	75.0	0	0	0	0	0
max.	100	2.3	3.8	1.9	8.9	13.3
	Mo	V	W	Al	Cu	Co
min.	0	0	0	0	0	0
max.	4.7	2.7	18.6	1.3	1.5	5.0

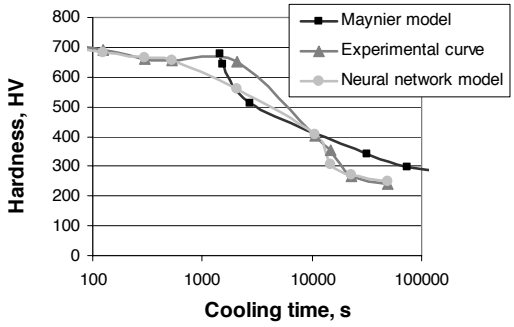


Fig. 4. Comparison of the calculated hardness change curves as function of cooling time with the experimental one for steels austenitised at 860ºC with concentrations of: 0.46% C, 0.77% Mn, 0.23% Si, 1.13% Cr, 1.49% Ni, 0.28% Mo, 0.18% V

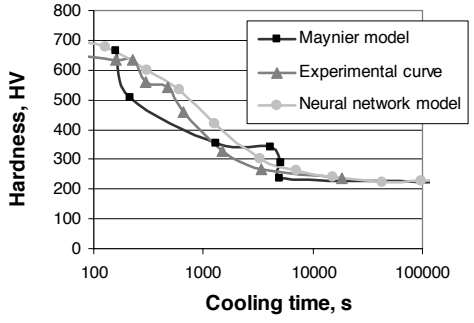
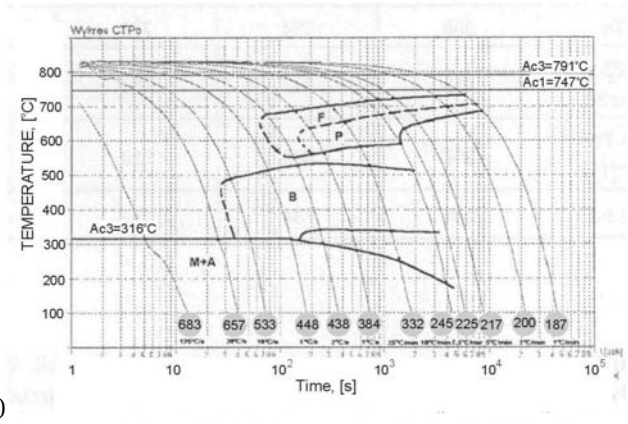


Fig. 5. Comparison of the calculated hardness change curves as function of cooling time with the experimental one for steels austenitised at 880ºC with concentrations of: 0.43% C, 0.82% Mn, 0.41% Si, 1.22% Cr, 0.04% Ni, 0.11% V

The purpose of the work [23] was to recognise the analytical potential of JMatPro software with relation to forecasting phase transformation diagrams. The results of CCT diagram simulation



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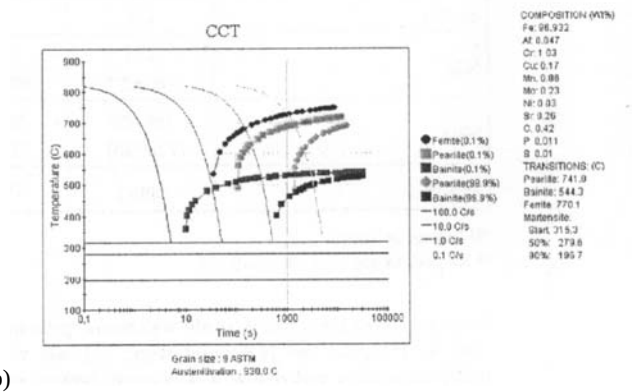

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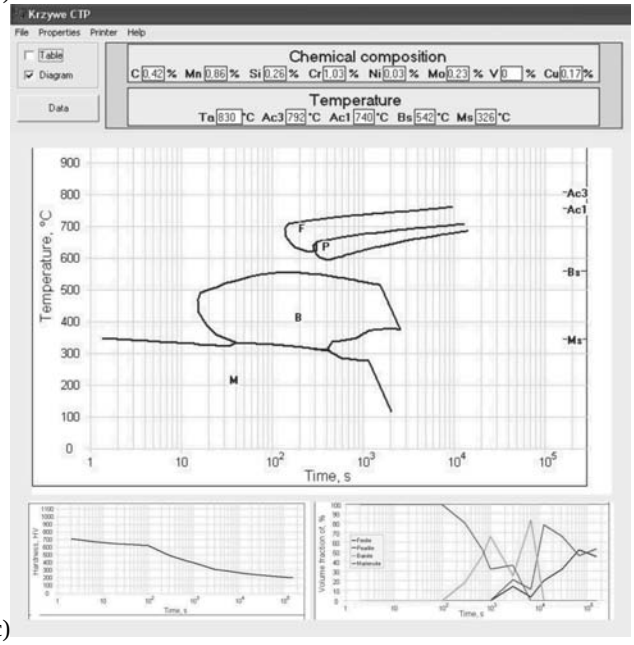
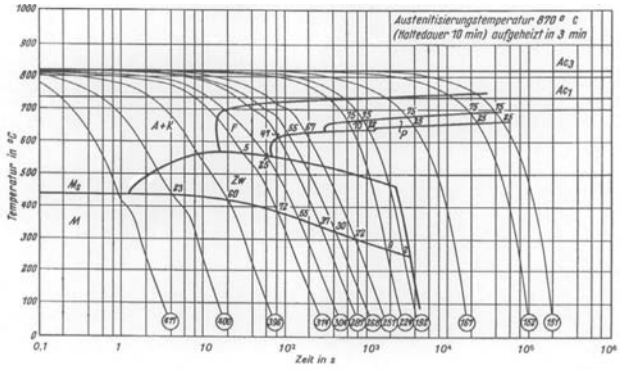


(c)

Fig. 6. CCT diagram for steel with concentrations: 0.42% C, 0.86% Mn, 0.26% Si, 1.03% Cr, 0.03% Ni, 0.23% Mo, 0.17% Cu, austenitised at 830°C: a) experimental [23], b) calculated using JMatPro software [23], c) calculated by the authors' method [11]



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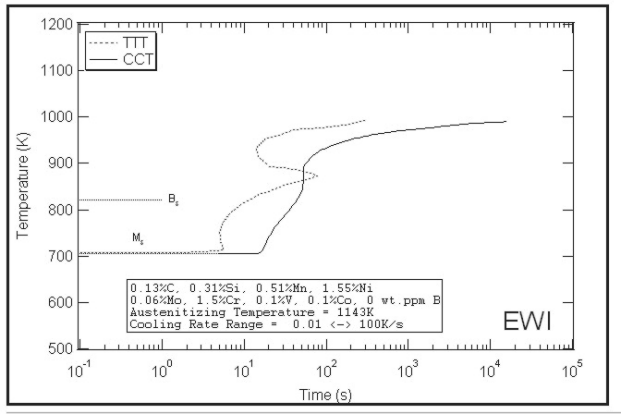

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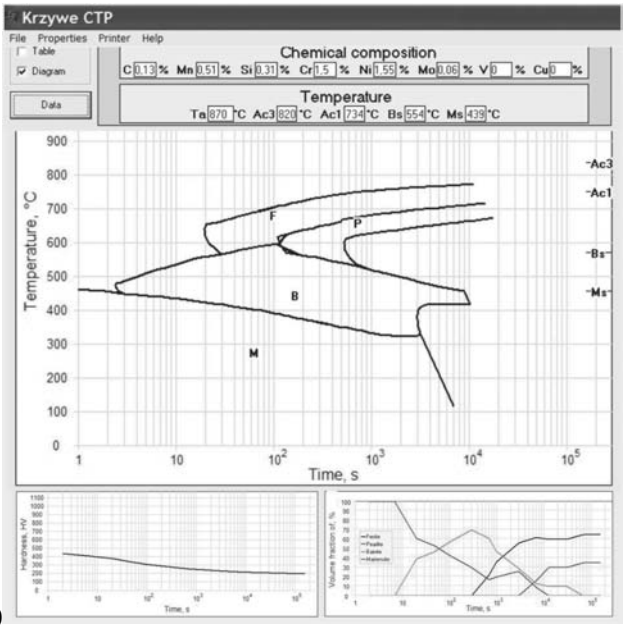

(c)

Fig. 7. CCT diagram for steel with concentrations: 0.13% C, 0.51% Mn, 0.31% Si, 1.5% Cr, 1.55% Ni, 0.06% Mo, austenitised at 870°C: a) experimental [13], b) calculated using EWI software [24], c) calculated by the authors' method [11]

using JMatPro software were compared to diagrams developed based on experiments using DIL 805 dilatometer. For expanding the scope of analysed steels calculations for phase change diagrams of materials with formerly developed CCT diagrams were carried out as well. Figure 6 presents graphical comparison of the CCT diagrams calculated using JMatPro software, authors' computer program and the experimental ones.

5. EWI software

Figure 7 presents graphical comparison of the CCT diagrams calculated using EWI (Edison Welding Institute) software [24], authors' computer program and the experimental ones.
The EWI computer program is available on the website at http://calculations.ewi.org/vjp/secure/TTTCCTPlots.asp. The online tool calculates and plots the TTT and CCT curves for the initiation (1%) of the transformation as a function of steel composition. Overall alloying element concentration should be less than 5%. The TTT diagrams are then used to calculate the continuous cooling transformation diagrams using the additivity rule. [25,26]]

6. Conclusions

The basis of a parameter selection many heat treatment operations is the knowledge of the supercooled austenite transformation kinetics during the continuous cooling from the austenitising temperature. The obtaining of the optimum properties of the steel is possible only after the application of suitable heat treatment and thermo-chemical operations or other technological processes (e.g. thermo-mechanical treatment). The proper selection of heat treatment parameters ensures also the optimum use of the alloying elements, what is extremely important when considering the economic criterion.

Fluctuations of the chemical composition of steel, allowable even within the same steel grade, and also changes of the austenitising conditions make that using the CCT diagrams published as catalogues does not provide reliable information on austenite transformations during cooling. The CCT diagrams which were determined by different institutes are markedly different. The interpretation of the dilatometer curves may vary from person to person.

The CCT diagram could be calculated using different methods. Some of them were presented in this paper. Calculation methods provide an alternative to experimental measurement in providing the material data required for heat treatment process simulation. The calculated properties can be used as an input to processing simulation packages like Finite Element Modelling tools.

The presented methods may be used for the selection of the chemical composition of the steel with the predetermined CCT diagram shape. [27,28]

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