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Project of computer program for designing the steel with the assumed CCT diagram

L.A. Dobrzański*, S. Malara, J. Trzaska
Division of Materials Processing Technology, Management and Computer Techniques in Materials Science, Institute of Engineering Materials and Biomaterials, Silesian University of Technology, ul. Konarskiego 18a, 44-100 Gliwice, Poland
* Corresponding author: E-mail address: leszek.dobrzanski@polsl.pl

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Analysis and modelling

ABSTRACT

Purpose: The aim of this paper was developing a project of computer aided method for designing the chemical composition of steel with the assumed CCT diagram.
Design/methodology/approach: The purpose has been achieved in four stages. At the first stage characteristic points of CCT diagram have been determined. At the second stage neural networks have been developed, and next CCT diagram terms of similarity have been worked out- at the third one. In the last one steel chemical composition optimization method has been developed.
Findings: The algorithm was created in this paper, that allowed to design the chemical composition of steel with the assumed CCT diagram.
Research limitations/implications: The created method for designing chemical compositions is limited by established ranges of mass concentrations of elements. The methodology demonstrated in the paper makes it possible to add new grades of steel to the system.
Practical implications: The method worked out may be used in computer steel selection systems for the machines parts exposed to heat treatment.
Originality/value: The presented computer aided method makes use of neural networks, and may be used for selecting the steel with the required structure after heat treatment.
Keywords: Computational material science; Artificial intelligence methods; CCT diagram

1. Introduction

Steels is the most commonly used material in today's engineering. The advantage of steels over other engineering materials lies in years of completed extensive research regarding its technological applications, and their influence on properties of materials, popularity and multiple applications, and the ability to use scraps as metallic charge in steel manufacturing process. The heat treatment process is often used to improve mechanical properties of constructional steel and engineering steel [1].

Continuous cooling transformation (CCT) diagrams are used in order to determine steel's properties like hardness, microstructure after hardening, tempering or full annealing. The diagrams show curves of the transformation-start temperatures (T_s) and transformation-finish temperatures (T_f) for all steel transformations with assumed chemical composition [1, 2–5]. Process of creating CCT diagram is very time-consuming and expensive. In order to reduce the necessary time and costs involved, a computer application was developed, which computes CCT diagrams for steels with assumed chemical composition. The application takes advantage of neural networks and extensive set of experimental data [6].

Artificial neural networks are systems that map the work of a human's brain. Processing capacity of computers is far more efficient than that of a human being, but a computer cannot learn by experiment, it cannot associate, predict, or make rational decisions. These properties are advantages of neural networks. The networks are built by many artificial neurons, which are connected by a net. Each neuron calculates the weighted sum of input signals and compares it to the threshold. Weights are determined by the process itself [7, 8].

Artificial neural networks are widely used in medicine, economy, engineering, and materials engineering [6, 9 – 15].

Currently, a reverse process to predicting the course of the supercooled austenite transformations is being developed with employment of neural networks. The purpose is to search for the chemical composition of steel with the assumed CCT diagram. The process causes difficulties, because one CCT diagram can correspond to many chemical compositions. The whole task is hard to complete, because it requires melting of steel with assumed chemical composition, and creating a CCT diagram by dilatometric methods. It is also difficult to define a numerical index of CCT diagrams similarity. Moreover, particular transformations can shift or disappear on the diagram, depending on chemical composition of steel.

2. Material and methodology

Steels for hardening and tempering were used to develop an application for designing the chemical composition of steel with the assumed CCT diagrams. Ranges of mass concentrations of elements are shown in Table 1.

Table 1.
Ranges of elements mass concentrations

	Elements mass concentrations (%)					
	C	Mn	Si	Cr	Ni	Mo
Minimum	0.076	0.00	0.12	0.00	0.00	0.00
Maximum	0.760	1.56	1.37	1.55	1.72	0.72

Algorithm used to develop a computer application is presented in Fig. 1. At first, 3000 random chemical composition were generated. For all generated compositions, CCT diagrams were computed by the computer program [6].

Terms of resemblance are difficult to formulate, which is the result of large number of data points on one CCT diagram. Preliminary computations were presented hereunder. An effort was undertaken to create system, which can determine CCT diagram in a clear-cut matter. A characteristic data was assumed and read from diagrams. The characteristic data was described as points, which were presented in Fig. 2.:

- for martensitic transformation:
  - temperature of start-transformation (point 1),
  - maximum time wherein transformation occurs (point 1);
- for bainitic transformation:
  - temperature of the smallest supercooled austenite life point (point 2),
  - time of the smallest supercooled austenite life point (point 2),
  - temperature of start-transformation at maximum time wherein transformation occurs (point 3),
  - maximum time wherein transformation occurs (point 3);
- for pearlitic transformation:
  - temperature of start-transformation at minimum time wherein transformation occurs (point 4),
  - minimum time wherein transformation occurs (point 4);
- for ferritic transformation:
  - temperature of start-transformation at minimum time wherein transformation occurs (point 5),
  - minimum time wherein transformation occurs (point 5).

At the next stage, ten neural networks were designed with employment of "Statistica Neural Networks 4.0 F" application. Each network computes a separate characteristic point. Neural networks quality was evaluated with three regression analysis components: mean absolute error, standard deviation for error and data and Pearson's correlation coefficient.

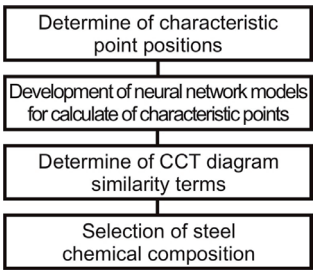

Fig. 1. Algorithm used to develop computer application

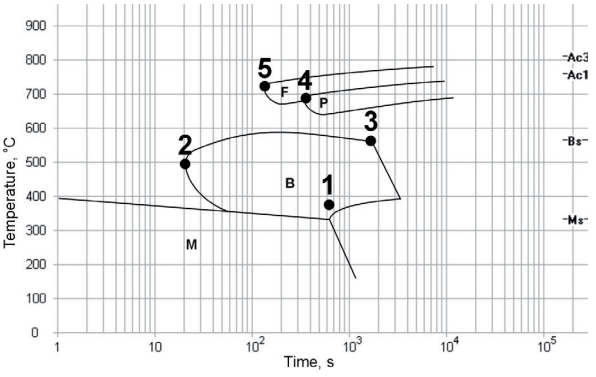

Fig. 2. CCT diagram with characteristic points marked

Data read from computed CCT diagrams was used in the design process. Data consisted of chemical compositions of steel (mass concentration of 6 elements) as input variables, and temperature, or time characteristic points, as output variable. Because of a significant difference between minimum and maximum values of data points (normalized time (t_p) was calculated by the following formula):

$$t_p = \sqrt[4]{t}\,, \tag{1}$$

where: t - time taken from CCT graphs,
t_p - normalized time.

Data set was divided into three subsets: training (1500 data), validating (750 data) and testing (750 data) ones.

Application, that computes chemical composition of steel with assumed CCT diagram, is based on an algorithm, presented in Fig. 3.

Chemical compositions are randomly generated (***A***) at the ranges of mass concentrations of elements shown in Table 1. Number of data set (random chemical composition) N is limited by the expected value of error E_u or by number of iteration. For each chemical composition, characteristic points are computed (***B***) and an error E is calculated (***C***). Total error E is a sum of relative errors δ_i for each of temperature and time value points (Fig. 2), and is given by:

$$E = \sum_{i=1}^{10} \delta_i \,. \tag{2}$$

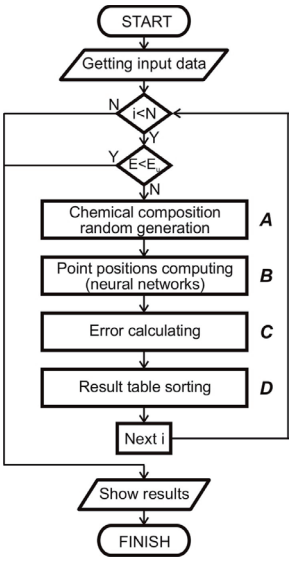

Fig. 3. Flow chart of algorithm for selection chemical composition of steel with assumed CCT diagram

Relative errors δ_i, for each of temperature and time computed value points x_{ci} related to expected value of time or temperature x_{ei}, are given by

$$, \delta_i = \frac{x_{ei} - x_{ci}}{x_{ei}} . \quad (3)$$

After total error calculations, chemical composition and total error values are added to the table, that stores chemical compositions with the best results. Every time a new chemical composition is added in, the table is sorted (***D***). The result of sorting is a table with chemical composition of steel the most matching the assumed CCT diagram.

3. Description of results

The result of design and optimisation process is set of ten neural network models, which are characterized by error of value, standard deviation and Pearson's correlation coefficient. The characteristics, that were a base of valuation, were presented in Table 2 and Table 3.

Pearson's coefficient of correlation is greater or equal to 0.98 for all but one neural networks computing values of normalized time, which points to a very strong relationship between actual and forecasted values.

Table 2.
Regression statistics of neural networks calculating normalized time values of characteristic points of CCT diagram in testing data set

Point no	Error, s	Standard deviation	Pearson's correlation coefficient r
1	0.19	0.21	0.98
2	0.07	0.15	0.99
3	0.22	0.15	0.99
4	0.16	0.16	0.99
5	0.34	0.56	0.83

Table 3.
Regression statistics of neural networks, calculating temperature values of characteristic points of CCT diagram in testing data set

Point no	Error, °C	Standard deviation	Pearson's correlation coefficient r
1	0.86	0.04	0.99
2	5.70	0.23	0.97
3	5.87	0.21	0.98
4	4.33	0.37	0.93
5	22.43	0.25	0.97

Quality of networks for calculated values of characteristic temperature points can vary. The highest quality is achieved for the network calculating the first point – start temperature of the martenistic transformation.). It's correlation coefficient values are close to 1 (0.99), which points to almost perfect estimates. The lowest quality network is the one computing temperature of pearlitic transformation (point 4). This result is most likely connected with inexistent pearlitic transformation for some chemical compositions of steel.

The developed computer application takes advantage of the algorithm (Fig. 3) which joins operations of all ten designed artificial neural network models. As a result, the application allows for designing of chemical compositions of steel with the CCT diagrams corresponding to the most accurate values. In the application, a user can assumed the position of all points, the number of chemical compositions, and expected values of the total error. Chemical compositions with values of total error are presented in a summary table. The application allows to save the results to a file in a form of a report. The application window is presented in Fig. 4.

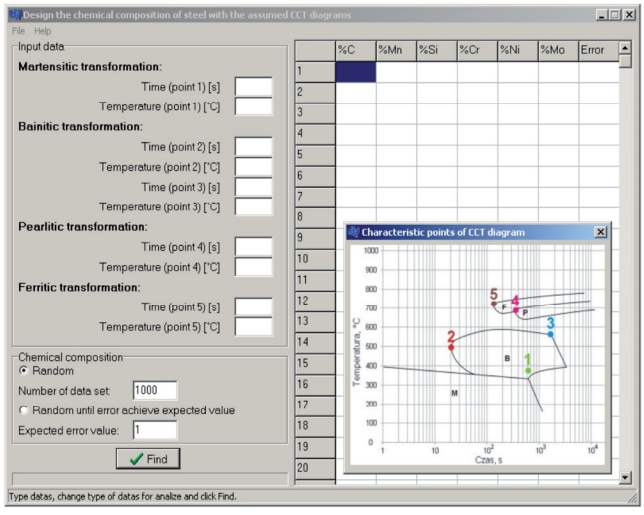

Fig. 4. Window of application for selection the chemical composition of steel with assumed CCT diagram

A solution to the hypothetical scenario for points in table 4 yields matching chemical composition of steel with the smallest value of the total error (table 5).

Table 4.
Demand characteristic points of CCT diagrams

Point no.	Value of time, s	Value of temperature, °C
1	50	290
2	2	400
3	40	550
4	30	650
5	7500	720

Table 5.
Computed steel chemical composition with errors

%C	%Mn	%Si	%Cr	%Ni	%Mo	Error
0.56	0.47	0.35	0.21	0.10	0.10	0.853

CCT diagrams corresponding to computed steel chemical composition is presented in Fig. 5.

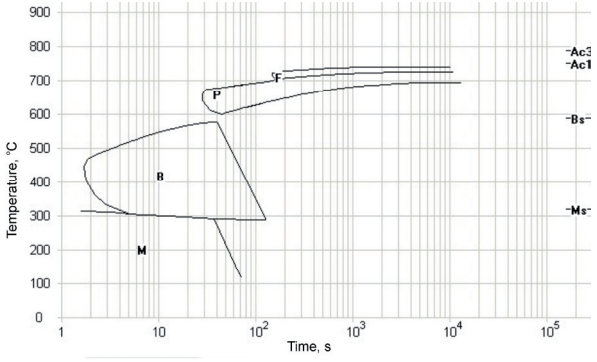

Fig. 5. CCT diagram for steel with concentrations: 0.56% C, 0.47% Mn, 0.35% Si, 0.21% Cr, 0.10% Ni, 0.10% Mo

4. Conclusions

This paper presents a project of computer program for designing of chemical composition of steel with assumed CCT diagram. The application is developed by selection of characteristic points for CCT diagrams, creation of neural network models, probability analysis, and proper optimization method. The application joins all ten artificial neural network models designed during the process and is an attempt to solve the reverse process to predicting the course of the supercooled austenite transformations. Because of a limited range of mass concentrations of elements for grades of steel for heat treatment, application's usability is limited and applied to developed neural network models only. To extend its use, an extension of the range of mass concentration is necessary. Other possibilities for enriching its use include selection of other alternative characteristic points of CCT diagrams. Implementation of these solutions, however, will result in a necessity to develop a better optimization algorithms, which add significant complexity. Another way to address the problem can be adding a range for all process changes during optimization (calculation of the total error).

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