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COMPUTER SOFTWARE FOR MODELLING CCT DIAGRAMS

OPROGRAMOWANIE KOMPUTEROWE DO MODELOWANIA WYKRESÓW CTPc

Abstract

The purpose of the paper is to present a computer program for calculating Continuous Cooling Transformation diagrams for constructional and engineering steels. The computer program uses artificial neural networks for prediction of steel parameters after heat treatment. Input data are chemical composition and austenitising temperature. The results of calculation consist of temperature of the beginning and end of transformation in the cooling rate function, the volume fraction of structural components and hardness of steel cooled from austenitising temperature at a fixed rate. The algorithm can be used in designing new chemical compositions of steels with required hardness after heat treatment.

Keywords: *computational material science, artificial intelligence methods, neural network, CCT diagrams*

Streszczenie

Celem niniejszego artykułu jest prezentacja komputerowego programu do obliczania diagramów CTPc dla stali konstrukcyjnych. Program ten korzysta ze sztucznych sieci neuronowych do predykcji parametrów stali po obróbce cieplnej. Danymi wejściowymi są skład chemiczny oraz temperatura austenityzowania. Wynikami obliczeń są temperatury początków i końców przemian w funkcji szybkości chłodzenia, udziały procentowe faz oraz twardość stali po chłodzeniu z temperatury austenityzowania. Algorytm może być użyty w projektowaniu nowych stali z wymaganą twardością po obróbce cieplnej.

Słowa kluczowe: *komputerowa nauka o materiałach, metody sztucznej inteligencji, sieci neuronowe, wykresy CTPc*

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1. Introduction

CCT diagrams are used for determination of the phase structure and hardness of steels after heat treatment like quenching, normalizing or annealing. The preparation of a CCT diagram for a steel with proper chemical composition requires a lot of experiments and very expensive testing equipment [1].

These are the main reasons for many attempts of modeling steel transformations during cooling. Many of these attempts involve mathematical models of processes proceeding in steel during cooling or empirical dependencies developed after many experiments.

Most equations are based on Jonson-Mehl or Avramy dependences. Some of them allow getting values of transformations temperatures, e.g. martensite start temperature. The obtained results of these equations in many cases are very different from real values of parameters. Most of them can be used only for a small group of steels with very similar chemical compositions. The transformations proceeding steel during heat treatment are very complicated therefore for modeling these processes artificial intelligence methods are used. Especially application of neural networks is very promising [2–4].

Some authors assume that application of a few simple neural networks instead of one big network allows calculation of required parameters with smaller errors [5–11]. This assumption is used in the presented computer program. The program calculates all parameters required for generating a CCT diagram, hardness of steel after cooling and phase structure of steel with chemical composition adopted by the user.

2. Program structure and algorithm of calculations

The computer program presented was developed in the Borland C++ Builder 6 programming environment. All neural networks were generated in Statistica Neural Networks 4.0 F computer program. Design of the proper neural networks required preparation of a representative set of data. This set of data was prepared from four hundred CCT diagrams published in the literature. The program cannot be used for any steel. The best results were obtained for the steels with ranges of mass concentrations shown in Table 1.

Table 1

Ranges of mass fractions of elements

	Mass fractions 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 works correctly only in Microsoft Windows operating system. The program consists of forty files, 21 of which are files with neural networks. The program has a modular structure shown in Fig. 1. Every unit contains a few files and performs a specific function.

The data input unit allows the user to input chemical composition and austenitising temperature for requested steel. Austenitising temperature can also be calculated by the program as temperature Ac3 + 50°C. The user can also input more than one chemical compositions of steel and save them in the file. It can be useful if a new version of the program appears and the user wants to compare the old and new results. All required data can be input using a user friendly form (Fig. 2).

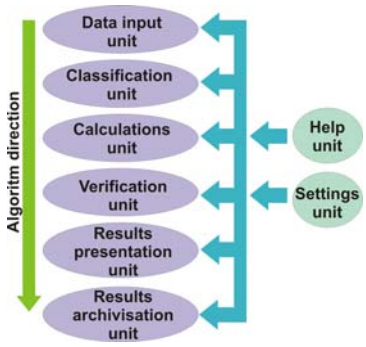


Fig. 1. Block diagram of the computer program

Rys. 1. Schemat blokowy programu komputerowego

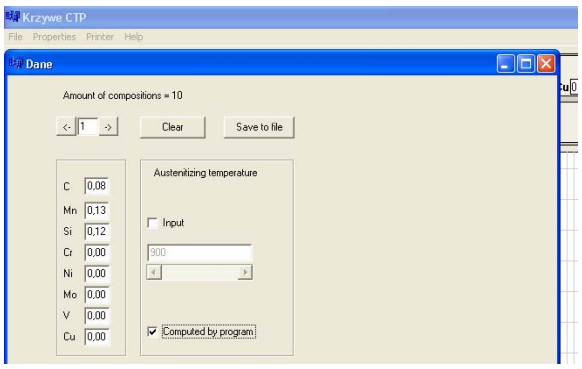


Fig. 2. Data input form

Rys. 2. Formularz wprowadzania danych

The classification unit consists of 4 files with neural networks: klasy_m.cpp, klasy_p.cpp, klasy_b.cpp and klasy_f.cpp. These neural networks (networks structures shown in table 3) are used to check whether the requested transformation is present during cooling at the adopted cooling rate. The first file contains functions to detect whether the ferritic transformation is present, the second for perlitic transformation, the third for bainitic transformation and the last one for martensitic transformation. Every file contains only neural networks. Therefore a fifth file was required for management of the aforementioned files. This file contains functions which:

– send starting parameters (chemical composition and austenitising temperature) for neural network inputs,
– run appropriate neural network,
– save results in to global table (Tab. 2).

These functions are run for every cooling rate (140 cooling rates were implemented).

Table 2

Global data structures

Global table	Content
Klasyf, klasyp, klasyb, klasym	Classifiers of transformations for all adopted cooling rates
Fstart, fkon, pstart, pkon, bstart, bkon, mstart	Start and finish temperatures of transformations calculated by neural networks for all adopted cooling rates
Fskon, fkkon, pskon, pkkon, bskon, bkkon, mskon	Start and finish temperatures of transformations after verification for all adopted cooling rates
Czasfsokr, czasfkokr, czaspsokr, czaspkokr, czasbsokr, czasbkokr, czasmsokr	Start and finish times of transformations for all adopted cooling rates
Bledy	Average errors values for the neural networks outputs
Procentfokr, procentpokr, procentfokr, procentmokr	Volume fractions of phases for all adopted cooling rates
Hv	Calculated hardness of steel for all adopted cooling rates
Ac1, ac3, ta, bsmax, msmax	Characteristic temperatures values calculated by the neural networks

The calculations unit consists of 17 files with neural networks. Also the management file was implemented. This file contains the following algorithm:
– send starting parameters (chemical composition, austenitising temperature and values of classifiers) for neural network inputs
– run appropriate neural network,
– save results in to global table (Tab. 2).

Running order of the neural networks is very important. The order is as follows:
– calculating the characteristic temperatures values (Ac1, ac3, ta, bsmax, msmax),
– calculating the values of the start and finish temperatures of transformations (ferritic, perlitic, bainitic, martensitic),
– calculating the start and finish times of transformations,
– calculating the hardness,
– calculating the volume fractions of phases.

The values calculated by neural networks must be verified, because in some cases the starting temperature of transformation can be lower than the finish temperature. Therefore a verification system was needed. For every temperature value calculated by neural networks a verifying function was implemented. These functions also save the results into global tables (Fskon, fkkon, pskon, pkkon, bskon, bkkon, mskon in Tab. 2). All verification procedures are shown in Fig. 3.

Table 3

Structures of the neural networks used for generating CCT diagram

Inputs	Neural network structure	Outputs
C,Mn,Si,Cr,Ni,Mo,V	7-4-1	The temperature of eutectiodal transformation A_{c1}
C,Mn,Si,Cr,Ni,Mo,V	7-5-1	The temperature of ferrit/austenit transformation A_{c3}
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta	9-8-1	The temperature of bainitic transformation B_{smax}
C,Mn,Si,Cr,Ni,Mo,V	7-6-1	The temperature of martensitic transformation M_{smax}
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-7-1	Classifier of the ferritic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-15-1	Classifier of the perlitic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-20-14-1	Classifier of the bainitic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-12-1	Classifier of the martensitic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-11-1	Start temperature of the ferritic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-7-1	Finish temperature of the ferritic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-5-1	Start temperature of the perlitic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-15-1	Finish temperature of the perlitic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,Bsmax,pierw	11-7-1	Start temperature of the bainitic transformation
C,Cr,Bsmax,Msmax,pierw	5-1250-5-1	Finish temperature of the bainitic transformation
C,Mn,Si,Cr,Ni,Mo,V,Cu,Ta,pierw	10-11-1	Start temperature of the martesitic transformation
Tempw,pierw	2-7-1	The times of start or finish transformation

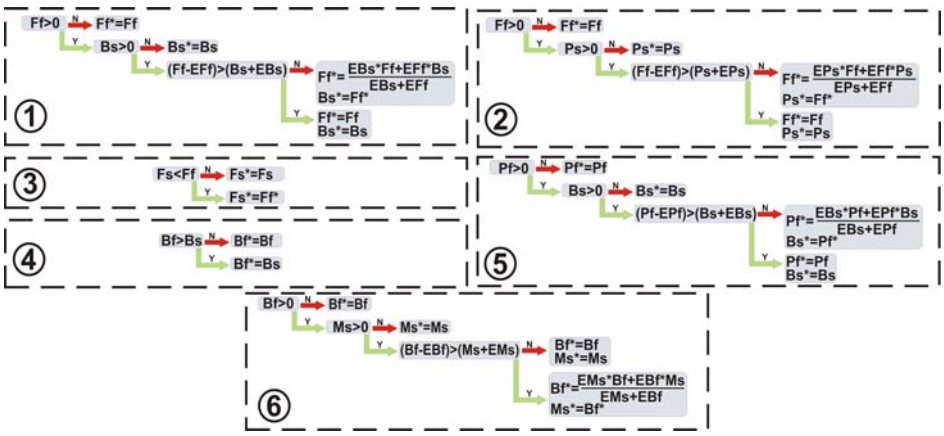
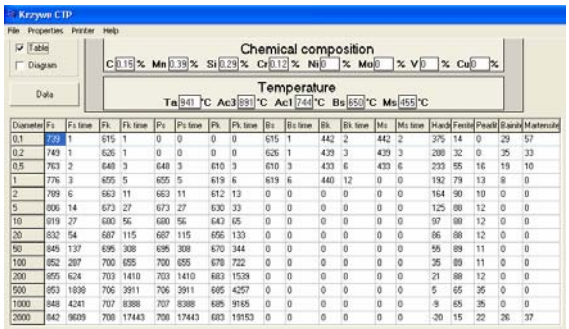


Fig. 3. The verification unit procedures

Rys. 3. Procedury modułu weryfikacji

The results presentation unit contains functions for generating a CCT diagram from the values calculated by the aforementioned units and placed in global tables. The results can be presented as a CCT diagram (Fig. 5) or as a results table (Fig. 4). Also hardness diagram and diagram of the volume fractions of phases are presented.



Diameter	Fs	Fs time	Fk	Fk time	Ps	Ps time	Pk	Pk time	Bs	Bs time	Bk	Bk time	Ms	Ms time	Hardn	Ferrite	Pearlite	Bainite	Martensite
0,1	739	1	615	1	0	0	0	0	615	1	442	2	442	2	375	14	0	29	57
0,2	749	1	626	1	0	0	0	0	626	1	439	3	439	3	288	32	0	35	33
0,5	763	2	648	3	648	3	610	3	610	3	433	6	433	6	233	55	16	19	10
1	776	3	655	5	655	5	619	6	619	6	440	12	0	0	192	79	13	8	0
2	799	6	663	11	663	11	612	13	0	0	0	0	0	0	164	90	10	0	0
5	806	14	673	27	673	27	630	33	0	0	0	0	0	0	125	88	12	0	0
10	819	27	680	56	680	56	643	65	0	0	0	0	0	0	97	88	12	0	0
20	832	54	687	115	687	115	656	133	0	0	0	0	0	0	86	88	12	0	0
50	845	137	695	308	695	308	670	344	0	0	0	0	0	0	56	89	11	0	0
100	852	287	700	655	700	655	678	722	0	0	0	0	0	0	35	89	11	0	0
200	855	624	703	1410	703	1410	683	1539	0	0	0	0	0	0	21	88	12	0	0
500	853	1838	706	3911	706	3911	685	4257	0	0	0	0	0	0	5	65	35	0	0
1000	848	4241	707	8388	707	8388	685	9165	0	0	0	0	0	0	-9	65	35	0	0
2000	842	9609	708	17443	708	17443	683	19153	0	0	0	0	0	0	-20	15	22	26	37

Fig. 4. The results table for calculated CCT diagram of a steel of the following chemical composition: 0,15% C, 0,39% Mn, 0,29% Si, 0,12% Cr

Rys. 4. Tabela wyników dla diagramu CTPc dla stali o składzie chemicznym: 0,15% C, 0,39% Mn, 0,29% Si, 0,12% Cr

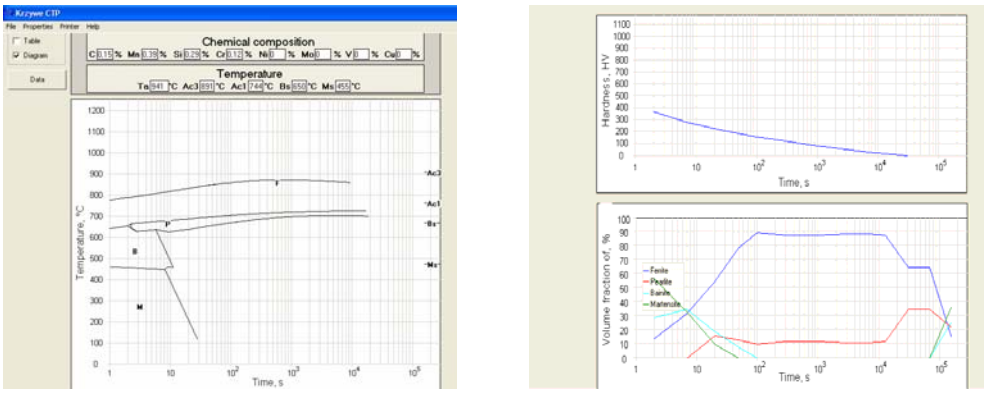


Fig. 5. The calculated CCT diagram, hardness diagram and volume fractions of phases diagram of the steel of the following chemical composition: 0,15% C, 0,39% Mn, 0,29% Si, 0,12% Cr

Rys. 5. Obliczone wykresy CTPc, twardości oraz udziału faz dla stali o składzie chemicznym: 0,15% C, 0,39% Mn, 0,29% Si, 0,12% Cr

The results archivisation unit allows the user to save the calculated results in a text file, save all the diagrams as a jpg image or send everything to printer. Saving process is fast and easy.

The help unit contains descriptions of all program functions, menus and settings.

The settings unit affects all unit. It allows language option (Polish or English), amount of input chemical compositions, precision of calculations, print settings and CCT diagram settings such as line thickness, or showing the calculated temperatures.

3. Results discussion

The data set (400 CCT diagrams) was divided into two parts. The first one was used for neural networks training. The second part of the data set was used only for evaluation of the

results obtained from neural networks. The obtained values of temperatures, times, hardness and volume fractions are very close to experimental data. Most of the average errors of the calculated parameters are lower than 5%. In Tab. 4 errors values for the calculated volume fractions of phases are shown. These results are acceptable. The calculated temperatures average errors are between 18 and 25 Celsius degrees (Tab. 5). Most of the Pearson coefficients for calculated parameters are close to 0,9. Also shape and position of the transformation curves are very similar to experimental diagrams (Fig. 6).

Table 4

Statistical coefficients of calculated volume fractions of phases

Variable	Average error [%]	Pearson coefficient
Ferrite volume fraction	5,2	0,88
Pearlite volume fraction	4,4	0,94
Bainite volume fraction	9,45	0,86
Martesite volume fraction	6,72	0,94

Table 5

Statistical coefficients of the calculated transformation start and finish temperatures

Calculated variable	Average error [ºC]	Average error [%]	Standard deviation of error [ºC]	Pearson coefficient
Fs	18,2	2,6	18,1	0,87
Ff	19,4	3,1	19,2	0,87
Ps	15,5	2,4	14,5	0,85
Pf	22,8	3,8	21,3	0,80
Bs	25,8	5,3	27,2	0,80
Bf	24,1	7,2	30,9	0,78
Ms	21,2	7,1	19,9	0,83

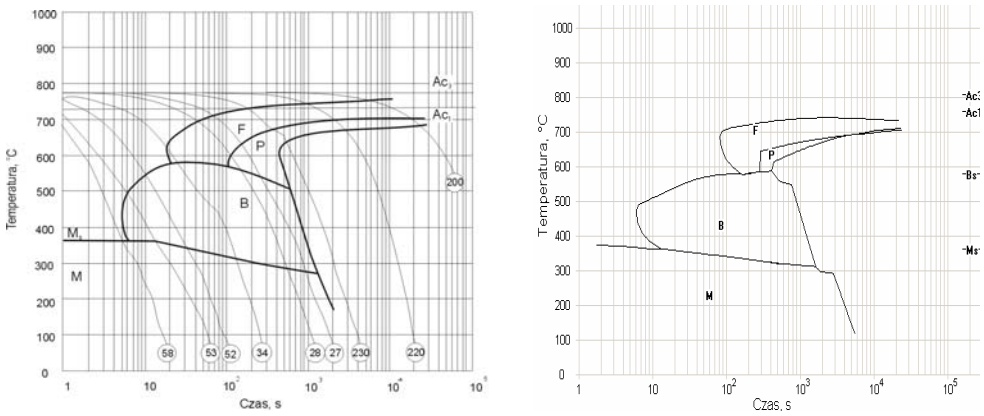


Fig. 6. The CCT diagram for steel of the following chemical composition: 0,38% C, 0,64% Mn, 0,23% Si, 0,99% Cr, 0,08% Ni, 0,16% Mo, 0,01% V, 0,17% Cu, austenitised in 1050ºC, a) experimental, b) calculated by program

Rys. 6. Wykres CTPc dla stali o składzie chemicznym: 0,38% C, 0,64% Mn, 0,23% Si, 0,99% Cr, 0,08% Ni, 0,16% Mo, 0,01% V, 0,17% Cu, austenityzowanej w 1050ºC, a) doświadczalny, b) obliczony przez program

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