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COMPUTER AIDED STEEL SELECTION FOR HEAT TREATED MACHINE ELEMENTS

Summary. In the present paper a structure and operation of expert system for selection of constructional steels being produced in Poland and EU countries and intended for quenched and tempered and thermo-chemical treated machine elements as well as for working out a technology of their heat and thermo-chemical treatment have been presented. Also the structure and operation of a program for calculation of hardenability - one of basic criteria for selection of alloy steels for quenched and tempered machine elements - which forms a set of calculating procedures being a part of the computer aided steel selection (CASS) has been described.

1. Introduction

Materials selection is an important part of designing process of machines and their elements. Just as for geometrical characteristic including dimensions and dimensional tolerance the design requires accurate determination of material properties such as e.g. steel grade, heat treatment and functional properties. Until now selection of materials, heat treatments and optimization of materials composition according to preselected criteria was carried out without the aid of a computer; it was open to subjective factors and often led to necessary mistakes or omissions of some criteria in multicriterial optimization of chemical compositions. In order to speed up the selection of constructional alloy steels for machine elements, to make objective the decisions related to the selection of chemical composition and to develop heat treatments considering among others best performance properties, the lowest possible heat treating costs and possible meeting other conditions, e.g. economical reasons, investigations were begun on a computer aided steel selection (CASS) with eventual aim of working out an expert system with the necessary data bases [1,2]. The general idea of the expert system for selection of steels intended for quenched and tempered and thermo-chemical treated machine elements as well as for working out the heat-, thermo-chemical treatment or surface technology was presented in another paper [2].

Detailed presentation of the program for calculation of the hardenability index of constructional alloyed and microalloyed steels, forming a part of the CASS system is the objective of the present work.

2. Structure and operation of CASS system

The general structure and operation chart is given in the fig. 1 and the complementary data in the table 1. More detailed description of the system is given in the paper [2].

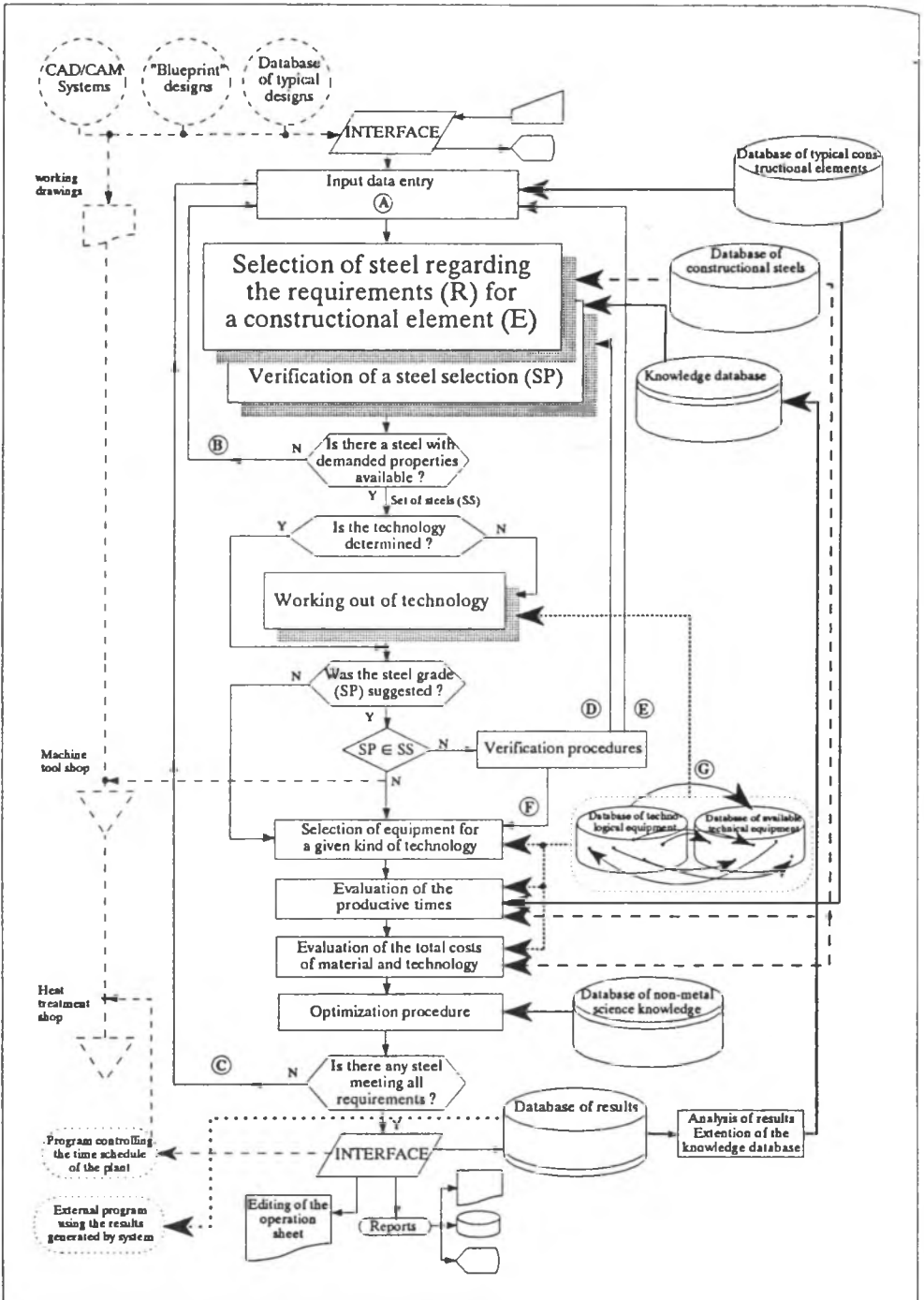


Fig. 1. Block diagram of the system structure and functions

Complementary data for the system structural chart presented in the fig. 1.

Designation	Description
A	Input data: obligatory: - type of element (E) with geometrical characteristics - requirements (R) concerning the steel properties - facilities and materials for heat treatment accessible for users optional: - steel grade (SP) proposed for production of the element - necessity of quality certification of the manufacturer - economical requirements - ecological requirements
B	The steel that would comply with the prescribed requirements does not exist in the steels data base
C	The result of optimization procedure is negative - no steel complying with all criteria has been selected. Necessary consultation and user decision concerning a change of some requirements and repetition of the procedure from the start point
D	Change of some parameters that do not require the user's decision
E	Suggestions to change the requirements when it is no longer possible to change parameters which do not need user's decision
F	Selection of proposed steel (SP) on the user's decision in spite of the negative verification of the steel by the system
G	In the stage of determining the input data, a base of facilities and technological means accessible for users is defined. Sometimes the user is interested in material selection with determination of the treatments and with consideration of all existing installations and materials. Then the base of facilities and technological means accessible for the user is the same as the base delivered with the system. If the user expects determination of the treatment with consideration of its accessibility to the installations and materials then the content of this base is determined by the user himself. The situation when the user has access to an installation not included in the base delivered with the system is also foreseen. Then ingoing base is enriched with this installation.

Among the basic functions performed by the system the following are included:

- selection of steel for heat treated and thermo-chemically treated structural parts with assurance of the required properties and compliance to other requirements and limitations given by designer, resulting from conditions of operation as well as from the accessibility of installations for heat treatments and from other economical and ecological criteria,
- working out the technology of heat- and thermo-chemical treatment incl. selection of processing operations, selection of temperature and time of quenching and tempering, cooling medium, conditions of thermo-chemical treatment etc.,

- substitution of a given steel by grades produced in other countries or included in ISO and CEN standards,
- calculation of heat and thermo-chemical treatment costs.

Moreover the system enables among others:

- calculation of hardenability indexes (critical diameter, hardenability band) on the ground of chemical analysis, grain size and cooling intensity,
- determination of mechanical, functional, physical and technological properties of steel according to the conditions of heat and thermo-chemical treatment,
- elaboration of steel specifications that are possible to use for particular constructional elements and specifications of elements that may be made from the given grade of steel.

Table 2

Examples of data taken from data bases

Data base	System function	Data
constructional steels	steel selection	hardenability band, carbon content, chemical composition, tensile strength, yield point, hardness, specifications of standards and steel grades used in Poland and EU countries, typical applications of steels
	process determination	upper and lower forging temperature, upper and lower temperature of soft annealing, upper and lower temperature of normalizing, upper and lower temperature of quenching in water and oil, upper and lower temperature of tempering for selected steel
	determination of material cost	price per weight unit
	determination of processing time	thermal conductivity coefficient, specific heat, density
typical constructional elements	determination of input data	types of constructional elements included in the base
	determination of processing time	important dimensions for determined type of constructional element (e.g. length, thickness, outside diameter, inside diameter) which enable the selection of heat and thermo-chemical treatment conditions
facilities and technological means	determination of technology	technical parameters of selected installation (e.g. capacity, efficiency, nominal power, idle power, energy for furnace heating up) characteristics of controlled atmospheres, characteristic of cooling media and solutions
	determination of processing time	technical parameters of selected installation (e.g. capacity, efficiency, rated power, idle power, energy for furnace heating up)
	determination of heat treatment costs	price of energy carriers, amortization

The system relies on extensive data bases of:

- constructional steels,
- typical constructional elements,
- technological facilities and media.

Examples of data used by various system procedures and taken from data bases are shown in table 2.

System knowledge, data base acquired from experts and created together with the system comprises a set of rules that enable the execution of its functions. Data introduced by the user and obtained as solutions of tasks are collected in the result data base and may be complementary for the system knowledge data base.

Calculation procedures for the system described in the paper [2] used for execution of particular utility functions of the system among things include calculation of hardenability indexes. System realizes its utility functions on the ground of input data given by the user incl. requirements resulting from conditions of operation and other accepted criteria.

Results of system operation are as follows:

- processing charts for heat and thermo-chemical treatment of constructional elements,
- complete or partial reports resulting from utility functions of the system or from calculation procedures also presented in the form diagrams,
- records in the result data base, making it possible to update knowledge data base and to cooperate with external programs.

Use of the system in conditions of an industrial plant is also foreseen. In this case input data may be incorporated as ready made designs of constructional elements prepared manually or using CAD and also as existing solutions collected in the base. In such case the role of the system is reduced to verification and confirmation of material selection and working out the heat, thermo-chemical or surface treatment procedures for a given element with consideration of optimizing criteria. Consideration of economical requirements is limited to checking out the costs of heat treatment.

The system provides also for communication with other programs, which may use its intermediate results. Among these programs one may mention:

- program for control of the production schedule in the company,
- accounting programs,
- other programs making use of data comprised in the result data base.

3. Structure and operation of the program for calculation of steel hardenability indexes

Hardenability is the basic criterion for alloy steel selection intended for quenched and tempered elements [3]. Hardenability as a technological property determines the ability of steel to harden and expresses the dependence of the maximal achievable hardness against austenitizing conditions and cooling rate [4]. For the classification purposes and to enable the use of hardenability while selecting the steels, a series of indexes and functions considered as hardenability measures are used, i.e.:

- 1) $HRC_j = f(x)$ – Jominy curve of a steel describing changes of Jominy hardness versus distance from the face,
- 2) D_{150-95} – the ideal critical diameter for various fractions of martensite in the section center,
- 3) D_{H50-95} – critical diameters for quenching media of different cooling intensities H with prescribed content of martensite in the section center.

The worked out program uses several dozen of procedures for calculation of different steel hardenability indexes. Functional relations of the procedures were taken either from the early works of Grossmann, Boyd & Field, Hodge & Orehsoki or Grossmann, Asimow and Urban, from standards ASTM 225 appendix X2, from Takashi Mori paper and from approximated relations given as tables or diagrams published by authors of this paper [5÷11]. These relations have the form of polynomials with coefficients given in the tables 3÷9.

Table 3

Polynomial coefficients applied in the procedures for calculations of DI_w for grain size $N = 7$.
General form of the function: $DI_w = A_0 + A_1 \cdot (\%C) + A_2 \cdot (\%C)^2$

Procedure No	Applicability limits %C	Coefficients		
		A_0	A_1	A_2
1	$C \leq 0,39$	0	0,54	0
2	$0,39 < C \leq 0,55$	0,171	0,001	0,265
3	$0,55 < C \leq 0,75$	0,115	0,268	- 0,038
4	$0,75 < C \leq 0,9$	0,062	0,409	- 0,135

The effect of alloying elements on the ideal critical diameter D_i is not influenced by the carbon content and grain size which do influence basic ideal critical diameter D_{iw} (related to the pure Fe-C alloy of specified grain size) [5]. The effect of grain size is considered by the relation for the basic critical diameter:

$$D_{iw} = 0,6(\%C)^{0,5} \exp(-0,816N) \quad (1)$$

which is valid for carbon contents up to 0,9% and for grain size in the range $N = 5$ to 8 [11]. The effect of alloying elements is to be determined by multipliers of the basic diameter:

$$D_{150} = D_{iw} \prod_{i=1}^n k_i \quad (2)$$

where:

D_{150} – the ideal critical diameter (the maximal diameter of the round bar quenched in ideal conditions, i.e. with the cooling intensity $H = \infty$) for at least 50% of martensite in the cross section center,

k_i – multiplier defining the influence of i -th alloying elements.

Dependence of these multipliers on alloying elements content is given in the diagrams [6].

On the ground of the calculated values of ideal critical diameter D_{150} one may determine the critical diameters D_{H50} for cooling media of the cooling intensity H from 0,01 to 10,0 by applying the relations given in the paper [7]. Additionally to determine the critical diameters for other fractions of martensite in the cross section centre (e.g. 80%, 90% and 95%) one may use the relations given in the paper [8].

Table 4

Polynomial coefficients applied in the calculation procedures k_{Mn} , k_{Si} , k_{Ni} , k_{Cr} , k_{Mo} , k_V , k_{Cu} , k_S , k_P .
General form of the function: $K_{(i)} = A_0 + A_1 \cdot (\%i) + A_2 \cdot (\%i)^2$

No of procedure	Element	Coefficients		
		A_0	A_1	A_2
5	Mn $\leq 1,2$	1	3,3333	0
6	1,2 < Mn $\leq 1,95$	-1,12	5,1	0
7	Si	1,0001	0,699986	0
8	Ni	0,989046	0,382183	0
9	Cr	0,999962	2,16	0
10	Mo	1,0	3,0	0
11	V	1,0	1,73	0
12	Cu	1,0016	0,362482	0
13	S	1,001	- 0,815	0,595
14	P	0,999	2,623	0

The ideal critical diameter can be used for calculation of Jominy curve [9], determination of steel hardness H_1 near the end of Jominy test specimen for various carbon contents and determination of dividing factors $DF = H_1/H_2$ which are used to calculate hardness at given distances to the specimen end.

Table 5

Polynomial coefficients applied in the calculation procedures for boron factor BF. General form of the function: $BF = A_0 + A_1 \cdot (\%C) + A_2 \cdot (\%C)^2 + A_3 \cdot (\%C)^3 + A_4 \cdot (\%C)^4 + A_5 \cdot (\%C)^5$

No of procedure	Range of application	Coefficients					
		A_0	A_1	A_2	A_3	A_4	A_5
15	AF ≤ 5	13,03059	-99,60059	374,8548	-707,3473	649,0013	-231,1499
16	5 < AF ≤ 7	10,29157	-69,64546	245,7061	-445,398	398,804	-140,6225
17	7 < AF ≤ 9	10,45573	-79,18535	311,9332	-630,549	627,6022	-244,4064
18	9 < AF ≤ 11	9,005326	-64,3767	249,6933	-506,0601	509,4772	-201,9323
19	11 < AF ≤ 13	8,054231	-55,1017	213,6752	-447,8863	477,8413	-204,4974
20	13 < AF ≤ 15	9,001262	-76,4768	355,871	-872,9646	1067,359	-512,7757
21	15 < AF ≤ 18	6,849017	-46,78647	196,6635	-471,3978	587,8504	-295,041
22	18 < AF ≤ 22	7,217034	-54,73529	248,9901	-632,7765	826,1873	-431,7227
23	22 < AF ≤ 26	7,162633	-57,52117	279,6173	-756,9353	1042,628	-568,568

Table 6

Polynomial coefficients applied in the procedures for calculation of determined hardness values H_1 , H_{50} . General form of the function:

$$H = A_0 + A_1(\%C) + A_2(\%C)^2 + A_3(\%C)^3 + A_4(\%C)^4 + A_5(\%C)^5$$

No of procedure	Value	Coefficients					
		A_0	A_1	A_2	A_3	A_4	A_5
24	H_1	35,395	6,99	312,33	-821,744	1051,479	-538,346
25	H_{50}	22,974	6,21	356,364	-1091,488	1464,88	-750,441

The method worked out by Grossmann [5] is used till now with modifications considering recent investigations, best developed in the method recommended by ASTM standard [10]. Full equation for calculation of the ideal critical diameter of a steel bar without additions of boron is as follows:

$$D_{150} = D_{1w} k_{Mn} k_{Si} k_{Ni} k_{Cr} k_{Mo} k_{Cu} k_V k_P k_S \quad (3)$$

The effect of boron is calculated using the boron factor (BF) whose value depends on carbon content and influences of alloying elements considered in the alloy factor (AF):

$$AF = D_{150}/D_{1w} = k_{Mn} k_{Si} k_{Ni} k_{Cr} k_{Mo} k_{Cu} k_V \quad (4)$$

One may calculate the values of BF, using the relation:

$$BF = A_0 + A_1(\%C) + A_2(\%C)^2 + A_3(\%C)^3 + A_4(\%C)^4 + A_5(\%C)^5 \quad (5)$$

Coefficients A_0 , A_1 , A_2 , A_3 , A_4 , A_5 depend on AF value and on carbon contents in steel. Exact BF values may be calculated only for standard accepted values of AF [10].

Consideration of boron effect on hardenability index values must be preceded by ensuring that all conditions of its effective work have been fulfilled:

- steel should be completely deoxidized and degassed [12],
- steel should contain elements assuring bonding of nitrogen - e.g. Al, Ti, Zr, [13,14],
- conditions of austenitizing should assure the optimal portion of boron in solid solution [14].

Hardness H_1 , achieved near the specimen end (initial hardness) and hardness of semimartensitic structure H_{50} for given steel is calculated from the relation:

$$H = A_0 + A_1(\%C) + A_2(\%C)^2 + A_3(\%C)^3 + A_4(\%C)^4 + A_5(\%C)^5 \quad (6)$$

Relations that enable the calculation of dividing factor DF, used for determination of Jominy curves are given in the standard [10].

ASTM standard [10] contains tabular specifications of all above mentioned coefficients. Calculations show, that many of the given equations result in not very exact approximations of the tabulated relations. Relations used in the procedure 1÷6, (table 3 and 4) have been accepted on the basis of equations given in ASTM standard [10]. Coefficients in the equations used in the

Table 7

Polynomial coefficients applied in the procedures for calculation of dividing factor DF.

General form of function: $DF = A_0 + A_1 \cdot D_1 + A_2 \cdot D_1^2 + A_3 \cdot D_1^3 + A_4 \cdot D_1^4 + A_5 \cdot D_1^5$

No of procedure	Distance from the sample end (mm)	Coefficients						Re-remarks	
		A_0	A_1	A_2	A_3	A_4	A_5		
26	3	1,55178	-0,026051	0,000429702	$-2,48638 \cdot 10^{-6}$	0	0	for steels without boron	
27	4,5	2,72229	-0,0768454	0,00118569	$-6,18321 \cdot 10^{-6}$	0	0		
28	6	4,52244	-0,157727	0,00282099	$-2,3052 \cdot 10^{-5}$	$7,10938 \cdot 10^{-8}$	0		
29	7,5	5,03965	-0,15632	0,00251526	$-1,90518 \cdot 10^{-5}$	$5,53032 \cdot 10^{-8}$	0		
30	9	4,16084	-0,078001	0,000678691	$-2,05388 \cdot 10^{-6}$	0	0		
31	10,5	4,33011	-0,0759589	0,000615213	$-1,74413 \cdot 10^{-6}$	0	0		
32	12	4,40247	-0,0749405	0,000590939	$-1,63955 \cdot 10^{-6}$	0	0		
33	13,5	4,5284	-0,0746598	0,000567732	$-1,51995 \cdot 10^{-6}$	0	0		
34	15	4,71993	-0,0774409	0,000581708	$-1,53896 \cdot 10^{-6}$	0	0		
35	18	4,94914	-0,0751432	0,000515341	$-1,24401 \cdot 10^{-6}$	0	0		
36	21	4,93379	-0,0687472	0,000433501	$-9,65664 \cdot 10^{-6}$	0	0		
37	24	5,03364	-0,068577	0,000428696	$-9,60879 \cdot 10^{-7}$	0	0		
38	27	5,06909	-0,0663788	0,000402862	$-8,90863 \cdot 10^{-7}$	0	0		
39	33	5,44541	-0,0706675	0,000418437	$-9,05402 \cdot 10^{-7}$	0	0		
40	39	5,57361	-0,0687932	0,000387464	$-8,04503 \cdot 10^{-7}$	0	0		
41	45	6,00671	-0,0766331	0,000441664	$-9,32747 \cdot 10^{-7}$	0	0		
42	51	6,37885	-0,082406	0,000472606	$-9,82001 \cdot 10^{-7}$	0	0		
43	3	1,36183	-0,011187	0,000111898	$-3,73023 \cdot 10^{-7}$	0	0		for boron containing steels
44	4,5	1,4905	-0,009841	6,04397	0	0	0		
45	6	25,1883	-1,65442	0,0456792	-0,000632738	$4,38249 \cdot 10^{-6}$	$-1,2117 \cdot 10^{-8}$		
46	7,5	20,2742	-1,06597	0,0236256	-0,000260039	$1,41631 \cdot 10^{-6}$	$-3,05042 \cdot 10^{-9}$		
47	9	12,0721	-0,436748	0,00655706	$-4,39764 \cdot 10^{-5}$	$1,10527 \cdot 10^{-7}$	0		
48	10,5	10,6698	-0,312724	0,00372816	$-1,90898 \cdot 10^{-5}$	$3,46194 \cdot 10^{-8}$	0		
49	12	9,59515	-0,240362	0,00237088	$-9,1925 \cdot 10^{-6}$	$9,84317 \cdot 10^{-9}$	0		
50	13,5	9,88284	-0,241898	0,00241183	$-1,01779 \cdot 10^{-5}$	$1,47362 \cdot 10^{-8}$	0		
51	15	10,6938	-0,265819	0,00275915	$-1,27058 \cdot 10^{-5}$	$2,16941 \cdot 10^{-8}$	0		
52	18	10,5618	-0,241675	0,00237205	$-1,05944 \cdot 10^{-5}$	$1,79908 \cdot 10^{-8}$	0		
53	21	11,3487	-0,242239	0,00223071	$-9,4654 \cdot 10^{-6}$	$1,54285 \cdot 10^{-8}$	0		
54	24	12,4325	-0,259918	0,00232433	$-9,52011 \cdot 10^{-6}$	$1,48406 \cdot 10^{-8}$	0		
55	27	13,6733	-0,28802	0,00259063	$-1,06832 \cdot 10^{-5}$	$1,67304 \cdot 10^{-8}$	0		
56	33	11,6207	-0,190815	0,001209	$-2,64714 \cdot 10^{-6}$	0	0		
57	39	12,802	-0,211513	0,0013536	$-3,00961 \cdot 10^{-6}$	0	0		
58	45	23,531	-0,562423	0,00563789	$-2,57754 \cdot 10^{-5}$	$4,43096 \cdot 10^{-8}$	0		
59	51	16,0087	-0,275556	0,00182459	$-4,19256 \cdot 10^{-6}$	0	0		

Table 8

Polynomial coefficients applied in the procedures for calculation of D_{in} for martensite fraction in the section centre $n = 80\%$, 90% , 95% .

General form of function: $D_{in} = A_0 + A_1 \cdot (D_{Iw}) + A_2 \cdot (D_{Iw})^2$

No of procedure	Martensite fraction in the section centre	Coefficients		
		A_0	A_1	A_2
60	95 %	1,775	0,786556	-0,00138986
61	90 %	1,56099	0,862068	-0,00117582
62	80 %	0,967033	0,938447	-0,00118931

Table 9

Polynomial coefficients applied in the procedures for calculation of D_H for selected cooling media of cooling intensity $H = 0,2$; $0,35$; $0,7$; 1 .

General form of function: $D_H = A_0 + A_1 \cdot (D_{Iw}) + A_2 \cdot (D_{Iw})^2 + A_3 \cdot (D_{Iw})^3$

No of procedure	Cooling intensity	Coefficients			
		A_0	A_1	A_2	A_3
63	0,2	-,0793114	0,119424	0,00370176	$-7,08864 \cdot 10^{-6}$
64	0,35	-1,39139	0,230859	0,00402278	$-8,00256 \cdot 10^{-6}$
65	0,7	-2,4996	0,378908	0,00461382	$-1,06665 \cdot 10^{-5}$
66	1,0	-2,89353	0,500249	0,00388165	$-9,40834 \cdot 10^{-6}$

procedures 7÷12 correspond to approximated tabulated functions from ASTM standard [10], checked and corrected in the present work. Relations used in the procedures 13 and 14 have been accepted after Takashi Mori [11]. Equations for BF, H_1 and H_{50} have been accepted acc. to ASTM standard [10] while the relations used in the procedures 26÷59 (table 7) have been worked out completely in the present work on the ground of tables in ASTM standard [10].

Appropriate approximation procedures for other values of alloy factor AF than that given in the table of ASTM standard, have been incorporated into the program for more exact calculation of boron factor BF.

Procedures Nos 60÷62 (table 8) for calculation of ideal critical diameters with fractions of martensite in the section centre other than 50% have been worked out on the ground of relations given by Hodge and Orehoski [8].

For calculation of critical diameters for selected cooling media of cooling intensity $H = 1,0$; $0,7$; $0,35$ and $0,2$ corresponding curves of the paper [7] have been described by the relations used in the procedures 63÷66 (table 9).

The program for calculation of hardenability indexes has been written using Borland C++ v.3.0. The results of its operation are written in a file named by the user while starting the pro-

gram. As the input data the steel composition is used (identified by the steel grade). Steel composition used for calculations is automatically recorded on the disc. While fixing the steel composition may be reproduced (if the steel has already been considered) and modified until accepted by the user. While the calculations of successive indexes are being performed the corresponding messages are displayed on the screen. The results of the program are accessible as disc file or may be printed on request. This information contains steel grade, chemical composition and calculated hardenability indexes.

To check the correctness of program operation some calculations of hardenability indexes for selected constructional alloy steels for quenching and tempering have been made, also for vanadium and boron microalloyed steels and the results obtained have been compared with published data [15÷20]. The average steel compositions have been taken for comparative calculations. The following alloy steels have been selected: 30G2 and 40HNMA [15,16], 28Mn6 and 51CrV4 [17], YF35MnV [18], WELDOX 900 and ABRAZO 40Q [19], TH 35 [20], SAE 15B30 [10].

The results of sample calculations presented in the paper [1] show good agreement with the data presented in the literature.

4. Final remarks

The philosophy and idea of an expert system for selection of constructional alloy steels being produced in Poland and EU countries and intended for quenched and tempered elements have been presented. As a result of system operation one may obtain technological charts for heat and thermo-chemical treatments as well as reports in the form tables and diagrams and data in the results base. For industrial applications the input data can be entered as ready designs of elements made by conventional methods or using CAD as well as collected in the data base of ready solutions. The system makes it possible to communicate with other programs for production management in a company. A program for calculation of steel hardenability indexes, comprising several dozen of calculating procedures, worked out and verified on the ground of published and standard data and taking into account the influence of carbon and alloying elements, various fractions of martensite in the section center, different cooling intensities and different primary austenite grain sizes forms a part of the system. Tabulated coefficients of verified relations have been given. Results of hardenability index calculations show good agreement with experimental data presented in the literature.

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