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CALCULATION OF CRITICAL TEMPERATURES BY EMPIRICAL FORMULAE

The paper presents formulas used to calculate critical temperatures of structural steels. Equations that allow calculating temperatures Ac_1, Ac_3, M_s and B_s were elaborated based on the chemical composition of steel. To elaborate the equations the multiple regression method was used. Particular attention was paid to the collection of experimental data which was required to calculate regression coefficients, including preparation of data for calculation. The empirical data set included more than 500 chemical compositions of structural steel and has been prepared based on information available in literature on the subject.

Keywords: CCT diagram, modeling, heat treatment, steel

1. Introduction

Empirical formulas that allow calculating critical temperatures in steel based on mass concentrations of elements have been presented in scientific publications for many years. To elaborate the equations the multiple regression method is used. In most cases the general linear form of the model was applied. Calculated values of regression coefficients pointed to the influence of elements on temperature. One of the first models was published in 1944 by Payson and Savage [1]. The researchers used some results of research by Greninger [2], which concerned the influence of carbon on the martensitic transformation start temperature Ms and the work by Greninger and Troiano [3]. The work also analysed the influence of other elements. The research was conducted for seventeen types of steel with a chemical composition specifically selected for tests. Payson's and Savage's equation coefficients were corrected sequentially by Rowland and Lyle [4], and Nehrenberg [5]. A similar form of equation was proposed two years later by Grange and Stewart [6] who analysed the data available at that time. In subsequent years, formulas that enabled calculation of other critical temperatures in steels were presented a number of times. Among many works on the subject, one that is worth mentioning is the publication by Steven and Haynes, wherein the effect of chemical composition on the Ms temperature and the bainitic transformation start temperature Bs was analysed [7]. In his work Andrews published formulas that enable calculating the start temperature for the transformation from pearlite into austenite (Ac_1), and the finish temperature for the transformation from ferrite to austenite (Ac_3) [8]. The issue of modelling critical temperatures in steels was analysed in detail in papers [9,10]. Many of the empirical formulas available in literature was collected in the paper [11]. Other methods were also used for modelling critical temperatures in steels. These included artificial neural networks [12-17].

The paper presents results of original work related to the modelling of critical temperatures in steels using the multiple regression method. Formulas presented in the paper [17] were modified. This was made possible thanks to supplementing the set of empirical data.

2. Data for calculations

In modelling using the multiple regression method it is very important to prepare a representative set of empirical data. Data preparation was begun with the selection of independent variables representing the model. The selection of variables is the result of the knowledge of the modelling process. However, the availability of data often requires the adoption of necessary simplifications. Vectors that contain examples used in modelling should include the values of all variables. Simultaneously, the values of explanatory variables should evenly cover the entire field of the approximated function. An analysis of the range of values of independent variables, in which the developed models can be used, was carried out. Assessment of the distribution of values of explanatory variables was made based on descriptive statistics, cluster analysis and histograms made for one or two variables. An example of a diagram showing scatterplot matrix for the Ac_3 temperature model is shown in the Fig. 1. For the same model, the Fig. 2 present examples of histograms showing the distribution of two elements: carbon and chromium as well as carbon and manganese.

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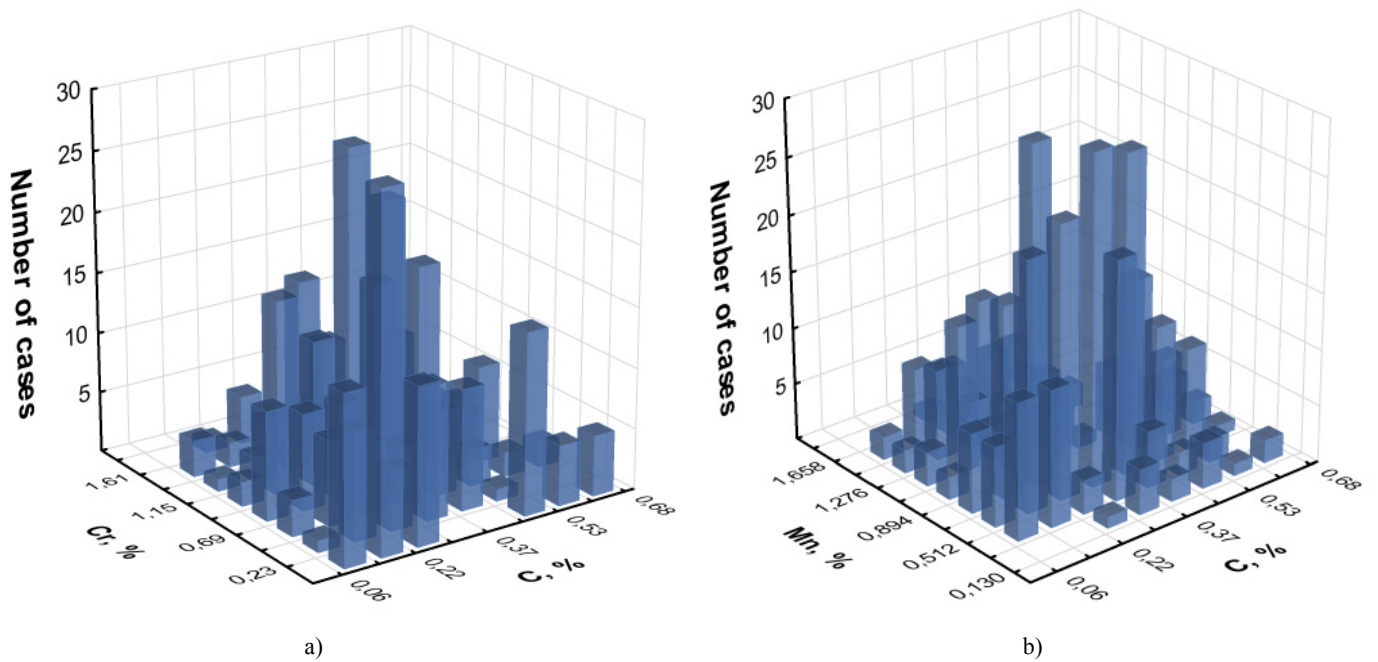Fig. 1. Scatterplot matrix for the Ac_3 temperature model

a)

b)

Fig. 2. Histograms showing the distribution of mass concentration of elements: a) carbon and chromium, b) carbon and manganese

Based on the conducted analyses the range of mass concentrations of elements, for which equation they can be applied, was determined. The minimum and maximum values are shown in Table 1. Moreover, additional conditions for the sums of concentrations of selected elements were defined (Table 2).

TABLE 1

Ranges of mass concentrations of elements

Range	Mass fractions of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
min	0.06	0.13	0.12	0	0	0	0	0
max	0.68	2.04	1.75	2.30	3.85	1.05	0.38	0.38
average	0.33	0.58	0.42	0.65	0.70	0.21	0.03	0.04
SD	0.13	0.37	0.37	0.54	1.02	0.24	0.07	0.07
SD – standard deviation								

TABLE 2

Additional conditions for limiting the scope of model application

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

Among other assumptions concerning the variables attention was paid to the collinearity of explanatory variables. An adverse effect of multicollinearity occurs when the explanatory variables are intercorrelated. The influence of the explanatory variable on the explained variable contains the influence of all variables correlated with it. Multicollinearity may cause a false assessment of the significance of independent variables of the model and change the symbol of the regression coefficient. Multicollinearity was assessed based on the correlation matrix for the model variables and the Variance Inflation Factor (VIF). VIF statistics (1) characterizes the increase in variance caused by correlating the analysed explanatory variable with other independent variables.

$$VIF_i = \frac{1}{1 - R_i^2} \qquad (1)$$

where:

R_i^2 – determination coefficient for the i-th independent variable, which acts as an explained variable in the auxiliary equation.

It is assumed that a moderate multicollinearity of explanatory variables occurs when the VIF $\geq$ 5, while in the case of VIF $\geq$ 10 strong multicollinearity is observed. [18] The values of the VIFs are summarized in Table 3. No multicollinearity was found for independent variables.

TABLE 3

The values of the Variance Inflation Factor

	Independent variables							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
VIF	1.13	1.34	1.11	1.26	1.26	1.15	1.15	1.05

3. Method and results

Work on each model was initiated by determining a mathematical form. A general form of the equation was accepted:

$$Y = a_0 + \sum_i a_i f_i(X) \qquad (2)$$

where:

Y – explained variable – transformation temperature;

$a_0, a_1 .. a_i$ – regression coefficients;

f_i – functions of equation variables;

X – vector of explanatory variables.

The equations were supplemented with additional components that took into account the interactions between explanatory variables. The interaction effect occurs when the influence of the explanatory variable on the explained variable changes with changes in the values of another explanatory variable. Products of two independent variables were introduced into the model. The estimation of regression coefficients for particular models was carried out using the least squares method.

Matching the equation to empirical data was assessed on the basis of the determination coefficient (R^2). The value of the determination coefficient allows estimating what part of variability of the dependent variable is explained by independent variables. Changes in the values of the determination coefficient also depend on the number of independent variables. Adding the variable to the model increases the value of R^2 even if the explanatory variable is useless in the model. Therefore, to assess the significance of explanatory variables that were added or removed from the equation, the value of the adjusted determination coefficient was used. The adjusted R^2 coefficient is carried out due to the number of degrees of freedom, i.e. the number of observations reduced by the number of independent variables. The adjusted determination coefficient allows comparing multiple regression models with different numbers of explanatory variables that have been developed for the same empirical data. The lower value of the adjusted coefficient from the R^2 value suggests that the model may contain an insignificant explanatory variable.

The significance of regression coefficients for the model was tested by verifying hypotheses concerning individual a_i coefficients in the form of a null hypothesis ($H_0: a_i = 0$), and an alternative hypothesis ($H_a: a_i \neq 0$). The Student's t-distribution was used to verify the hypotheses. The testing statistics was calculated as the quotient of the regression coefficient and the standard error for this coefficient. The level of significance was $\alpha = 0.05$. When the null hypothesis was rejected, the regression coefficient for the explanatory variable was considered statistically different from zero, assuming that the independent variable is statistically significant and influences the explained variable. The null hypothesis was rejected when the p-value, which was the calculated significance level for the testing statistics t, reached a lower value than 0.05. Insignificant variables were removed from the equation, and then the regression coefficients were calculated once more.

Values of statistics for temperature models: Ac_1, Ac_3, B_s and M_s are presented in Table 4. Table 4 shows the final part of the analysis after removing the insignificant variables.

TABLE 4

Values of statistics used to evaluate the significance
of regression coefficients

Variable	Int.	C	Mn	Si	Cr	Ni	Mo	V	Cu
Model	Ac_1								
RC	741.9	–29.1	–14.0	12.6	15.9	–16.8	–16.2	45.2	36.3
Standard error	3.5	5.7	2.2	2.0	1.4	0.8	3.1	11.3	9.8
t Stat	212.3	–5.1	–6.4	6.4	11.0	–21.9	–5.2	4.0	3.7
p–value	0	5E–7	4E–10	4E–10	2E–25	7E–75	2E–7	8E–5	2E–4
Model	Ac_3								
RC	924.7	–219.4*	–6.9	39.2	–	–15.9	13.4	97.0	–
Standard error	5.2	7.3	2.5	2.3	–	0.9	3.5	13.6	–
t Stat	176.4	–29.9	–2.8	16.7	–	–18.1	3.8	7.1	–
p–value	0	3E–111	0.006	2E–49	–	4E–56	0.0001	4E–12	–
Model	B_s								
RC	770.9	–231.5	–68.7	–23.3	–58.5	–30.8	–55.4	–41.3	–
Standard error	6.9	10.6	4.1	3.6	2.6	1.4	5.4	19.8	–
t Stat	112.4	–21.9	–16.8	–6.5	–22.3	–22.3	–10.3	–2.1	–
p–value	0	1.1E–7	6E–50	2E–10	2E–75	2E–75	1E–22	0.04	–
Model	M_s								
RC	541.2	–401.2	–35.6	–10.5	–14.2	–18.1	–17.1	–	–
Standard error	4.7	7.6	2.9	2.4	1.8	0.9	3.4	–	–
t Stat	115.8	–52.6	–12.3	–4.4	–7.7	–18.7	–5.01	–	–
p–value	0	8E–205	2E–30	1E–05	5E–14	1E–59	7E–7	–	–

$*\ \sqrt{C}$; Int. – Intercept; RC – regression coefficient

The statistical significance of the regression model was examined using the F test. The testing statistic with the F-Fisher-Snedecor distribution was calculated as the quotient of the mean value of the regression squares, and the mean square error taking into account the degrees of freedom. The null and alternative hypotheses were verified. Accepting the null hypothesis means that there is no dependence between the set of explanatory variables and the explained variable. The alternative hypothesis for the F test that confirmed the statistical significance of at least one regression coefficient was assumed when the p-value was lower than 0.05. Table 5 summarizes the statistics for the F test supplemented with, among others, the values of the standard error, the correlation coefficient (R), the determination coefficient R^2 and the adjusted determination coefficient.

TABLE 5

Values of statistics used to evaluate the significance
of the developed models

	Model			
	Ac_1	Ac_3	B_s	M_s
R	0.78	0.86	0.87	0.93
R^2	0.61	0.75	0.75	0.87
Adjusted R^2	0.61	0.75	0.75	0.86
Standard error	15.55	17.80	27.53	19.99
Observations	500	484	476	502
Significance F	1.14E–96	3E–140	9E–138	1E–212

The elaborated models were also assessed on the basis of: the mean absolute error, the standard error deviation, and the standard deviation quotient of the calculation error, as well as the standard deviation of the dependent variable value. The standard deviation quotient allows referring the error value of the model to the scope of changes of the dependent variable. The „ideal" value for this statistic is 0.

Table 6 shows the following values: the mean absolute error, the standard error deviation, and the standard deviation quotients for error and empirical values of the dependent variable.

TABLE 6

Values of statistics used to evaluate the quality
of the developed models

	Mean absolute error, °C	Standard deviation of the error, °C	Ratio of standard deviations
Ac_1	12.4	9.2	0.36
Ac_3	14.1	10.7	0.30
B_s	21.2	17.2	0.31
M_s	14.8	13.3	0.24

When applying the presented procedure, equations that explain the dependence between the chemical composition of steel and transformation temperatures were elaborated: Ac_1, Ac_3, B_s and M_s. Critical temperatures models are shown in equations (3)-(6).

$$Ac_1 = 742 - 29 \cdot C - 14 \cdot Mn + 13 \cdot Si + \\ + 16 \cdot Cr - 17 \cdot Ni - 16 \cdot Mo + 45 \cdot V + 36 \cdot Cu \tag{3}$$

$$Ac_3 = 925 - 219 \cdot \sqrt{C} - 7 \cdot Mn + \\ + 39 \cdot Si - 16 \cdot Ni + 13 \cdot Mo + 97 \cdot V \tag{4}$$

$$B_s = 771 - 231.5 \cdot C - 69 \cdot Mn - 23 \cdot Si \\ - 58,5 \cdot Cr - 31 \cdot Ni - 55 \cdot Mo - 41 \cdot V \tag{5}$$

$$M_s = 541 - 401 \cdot C - 36 \cdot Mn \\ - 10,5 \cdot Si - 14 \cdot Cr - 18 \cdot Ni - 17 \cdot Mo \tag{6}$$

For critical temperature models the following scatter plots for dependent variable values that were experimental and calculated using equations (3-6) were made. The results are shown in Fig. 3.

4. Summary

The paper presents equations describing the dependence between the chemical composition of steel and the start temperature for the transformation from pearlite into austenite (Ac_1), the finish temperature for the transformation from ferrite into austenite (Ac_3), the bainitic transformation start temperature (B_s), and the martensitic transformation start temperature (M_s).

The theory of correlation and regression is a useful tool to determine the degree of connection of variables in a model. It allows answering the question whether there is a dependence
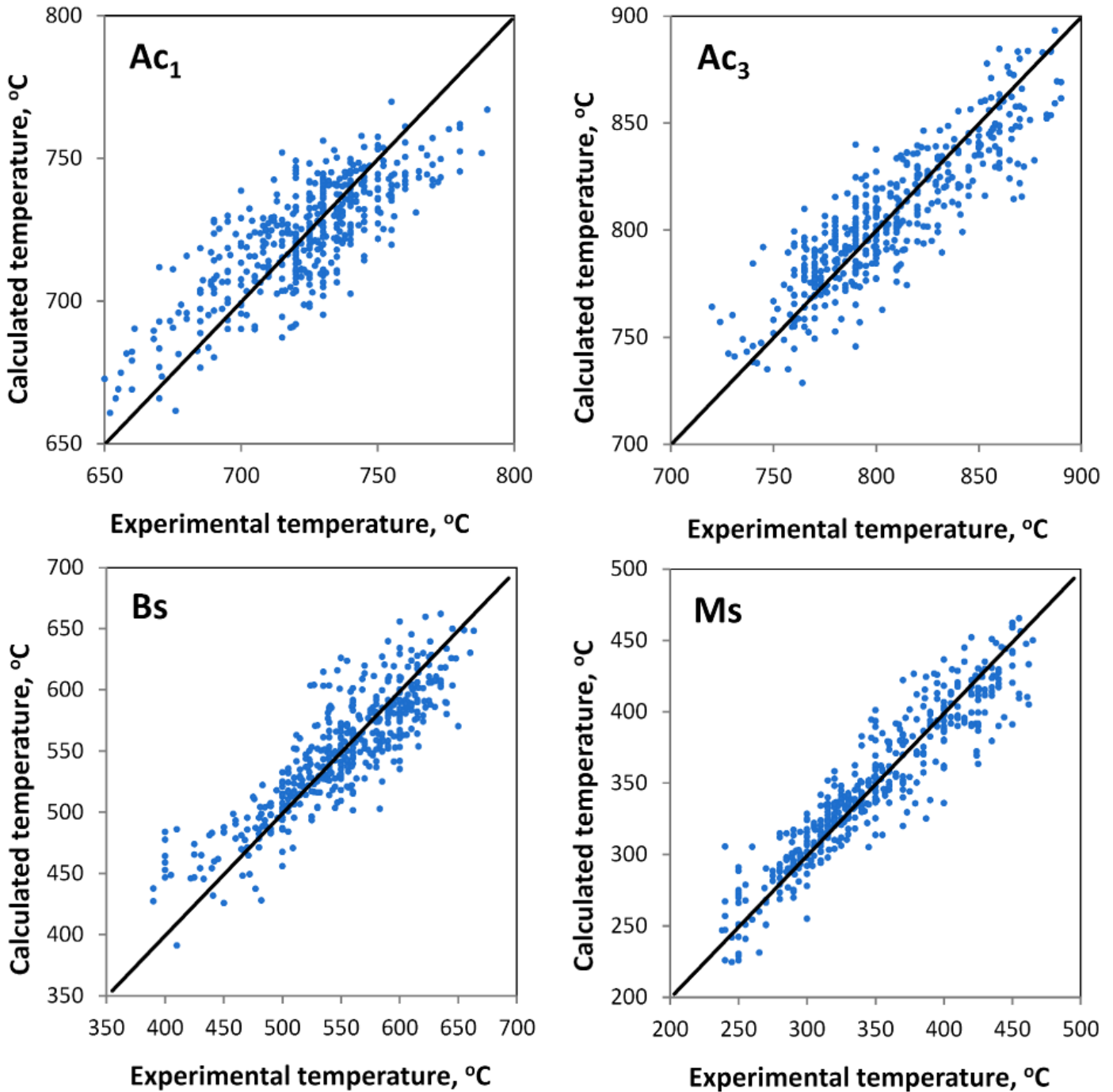
Fig. 3. Comparison of the experimental temperatures with values calculated using the regression model

between variables and whether it is close. Moreover, the equations can be easily spread and widely used, as well as verified by other research results. A certain piece of information on the dependence between the explanatory variables and the explained variable is visible in the form of values of coefficients of the regression equation. The value of the regression coefficient may not always be interpreted as the force of influence of an element on the value of transformation temperature. It should be remembered that there is variability in the explanatory variable and the values of other independent variables.

The set of empirical data has essential meaning for the quality of the developed models. The set was used to calculate the regression coefficients. The presented equations can be used only in the range of concentrations of alloying elements shown in the Table 1. Simultaneously, the conditions set out in the Table 2 should be complied with.

The multiple regression and logistic regression methods were also used to develop other models that describe the transformation temperatures as a function of the cooling rate, hardness of steel and volume fractions of ferrite, pearlite, bainite and martensite in the microstructure of steel. The results are shown in papers [19-21].

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