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J. TRZASKA*,#

# EMPIRICAL FORMULAS FOR THE CALCULATIONS OF THE HARDNESS OF STEELS COOLED FROM THE AUSTENITIZING TEMPERATURE

In this paper, the equations applied for the purpose of the calculations of the hardness of continuously cooled structural steels upon the basis of the temperature of austenitizing. The independent variables of the hardness model were: the mass concentrations of elements, the austenitizing temperature and the cooling rate. The equations were developed with the application of the following methods: multiple regression and logistic regression. In this paper, attention was paid to preparing data for the purpose of calculations, to the methodology of the calculations, and also to the assessment of the quality of developed formulas. The collection of empirical data was prepared upon the basis of more than 500 CCT diagrams.

*Keywords*: CCT diagram, modeling, heat treatment, steel, hardness

## 1. Introduction

Computer-assisted modelling is more and more frequently taken advantage of in materials engineering. Theoretical predictions, supported by computer-assisted methods, are complemented by empirical methods. That is relevant to predicting the properties of materials, introducing new materials and the technologies of manufacturing them, and also to optimizing those already existing materials and processes. [1-6]

The diagrams of the transformations of supercooled austenite for continuous cooling (CCT) are developed in laboratories in numerous countries, and published in atlases, handbooks and scientific publications. As well as those, there are models describing the influence exerted by chemical composition upon the temperatures of transformations, hardness, and also the volume fraction of ferrite, pearlite, bainite and martensite in the microstructure of steels. [7-10] A popular method of modelling in this area is multiple regression. [11,12] Empirical formulas constitute the basis of the algorithms applied in computer programs serving for the purpose of the calculations of the CCT diagrams.

A popular model taken advantage of in numerous applications for the purpose of the calculations of microstructural constituents and the hardness of a continuously-cooled steel from the austenitizing temperature is the Maynier model [13,14]. In that model, the following were taken under consideration: the influence exerted by the chemical composition of a steel, and also the temperature and the time of austenitizing. The Maynier equations make it possible to calculate the typical cooling rates at the temperature of 700 degrees Celsius, for which in the microstructure of steels the following quantities are formed: 100%, 90% and 50% of martensite, 90% and 50% of bainite, and also 90% and 100% of ferrite and pearlite (respectively). The Maynier model was developed upon the basis of the data acquired from approximately 300 CCT diagrams. In the literature, there are as well examples of the calculations of the hardness of a continuously-cooled steel upon the basis of the Jominy hardenability curve [15] and [16] that are presented.

The first results of own research connected with modelling the hardness of steel cooled from the austenitizing temperature were presented in the papers [17,18]. For the purpose of developing the hardness model, the method of artificial neural network was applied. In the paper [19], equations for the purpose of the calculations of the transformations temperature of supercooled austenite developed with the application of the multiple regression method were presented. In spite of an attempt made back then, it proved to be impossible to develop the adequate hardness model. A significant improvement of the results was achieved no sooner than when additional dichotomous variables, which represented the constituents of the microstructure of a steel in the form of ferrite, pearlite, bainite and martensite, were introduced in the equation. The calculations of the values of those variables required developing the classificators with the application of the logistic regression method. The model of the steel hardness in which dichotomous variables were applied, was presented in the paper [20].

Complementing and extending the collection of empirical data made it possible to develop new equations connecting the chemical composition of a steel, the cooling rate and the austenitizing temperature with the hardness of a steel. In the paper, the following equations were presented: making it possible to estimate the hardness of continuously-cooled steel from the austenitizing temperature, and also the modified versions of equations for the purpose of the calculation of the kinds of the microstructural constituents of a steel.

* SILESIAN UNIVERSITY OF TECHNOLOGY, INSTITUTE OF ENGINEERING MATERIALS AND BIOMATERIALS, 18A KONARSKIEGO STR., 44-100 GLIWICE, POLAND

# Corresponding author: jacek.trzaska@polsl.pl

## 2. Data for calculation

Modelling hardness with the application of the multiple regression method required preparing a representative set of empirical data. The collection of data has to be a collection typical for the process being modelled. The values of independent variables ought to uniformly cover the entire domain of the function being approximated. The selection of independent variables ought to result, first and foremost, from the knowledge relevant to the process being modelled. In numerous cases, however, it is necessary to simplify the model, and that results, among others, from the availability of empirical data.

The data set was developed upon the basis of atlases, handbooks and scientific publications containing experimentally-determined CCT diagrams. More than 500 CCT diagrams for structural steels were taken advantage of. The information connected with the austenite grain size and the austenitizing time was not provided on the majority of the CCT diagrams. For that very reason, it was necessary to adopt simplifications connected with the number of independent variables describing the model. It was presumed that the independent variables of the model would be the mass concentrations of the following elements: C, Mn, Si, Cr, Ni, Mo, V and Cu, the cooling rate, and also the austenitizing temperature. Upon the basis of one CCT diagram, several vectors containing the values of independent variables and the respective value of hardness were developed. The data set applied for the purpose of developing the model contained 2845 cases. In addition to that, a verification data set was separated, and that data set was taken advantage of for the purpose of the numerical verification of the model. The verification data set contained 300 cases.

The statistical assessment of the data set was performed upon the basis of descriptive statistics. For every variable of the model, the following statistics were analysed: the minimum value, and the maximum one, mean, standard deviation, median, kurtosis and skewness. The scatterplot matrix and histograms were developed for every independent variable, and so were histograms for two variables. It was checked if there were outliers occurring in the data set. What was analysed as well was the multicollinearity of independent variables. For the purpose of analyzing the effect of multicollinearity, the correlation matrix was taken advantage of, and the values of VIF (Variance Inflation Factor) were calculated as well. Upon the basis of the conducted analyses, the scope of mass concentration of elements, for which the equations may be applied, was determined. The minimum value, and the maximum one, were presented in Table 1. As well as those, the additional conditions, relevant to the sums of the 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 |

## 3. Method and results

In the hardness models developed with the application of the artificial neural networks method [9,17], the significant variables were constituted by dichotomous variables describing the occurrence of: ferrite, pearlite, bainite and martensite in the microstructure of a steel. For the purpose of the calculation of those variables, the classificator developed with the application of the artificial neural network method was applied. Independent variables in the model were constituted by the mass concentrations of elements, the austenitizing temperature and by the cooling rate. The first classificators developed with the application of the logistic regression method were presented in the paper [20]. The corrected versions of the equations which were taken advantage of in this paper as well were presented in the paper [21]. The above-mentioned classificators are the important part of the hardness model, and, for that very reason, they were included in this paper (Eq. (1)-(6)).

The regression coefficients of classificators were estimated with the application of the maximum likelihood method [22]. That method does not provide an analytical solution. Numerical solutions are based upon the multiple estimation of regression coefficients in order to obtain results similar to those in a given sample. For the purpose of the calculations of regression coefficients, the Rosenbrock method and the quasi-Newton one were applied. The significance of independent variables was assessed taking advantage of the Wald test. The basis for recognizing the significance of the variable statistical describing was rejecting the null hypothesis. The test statistic $Z^2$ was calculated as the square of quotient of regression coefficient for an analysed explanatory variable and a standard error for that coefficient. The distribution of statistic $Z^2$ is in accordance with the distribution of $\chi^2$ with one degree of freedom. The null hypothesis was rejected if the p-value, being the calculated level of significance for the test statistic $Z^2$, was smaller than the presumed level of significance $\alpha=0.05$.

It was presumed that the dichotomous dependent variable Wx (Eq.(1)), describing the occurrence in the microstructure of the steels of the following: ferrite, pearlite, bainite and martensite, assumes the value of 0 (the constituent does not occur in the microstructure of a steel), if calculated with the application of equation (2) the value of variable Sx is not greater than a certain threshold value (N). The threshold value was determined by means of minimizing the number of incorrect answers.

$$W_X = \begin{cases} 0 \; dla \; S_X \leq N \\ 1 \; dla \; S_X > N \end{cases} \tag{1}$$

$$S_X = \frac{\exp(K_X)}{1+\exp(K_X)} \tag{2}$$

where:
X=f (ferryt), p (perlit), b (bainit), m (martenzyt),
N= 0.5 for ferritic, pearlite and martensitic transformation; N=0.4 for bainitic transformation.

Equations (1) and (2), and also (3)–(6), make it possible to estimate whether in the microstructure of a steel cooled at a certain rate from the austenitizing temperature, the following: ferrite, pearlite, bainite and martensite are observed. In the case of ferritic transformation (3) and the pearlite one (4), the issue can be reduced to searching for the highest cooling rate which is sufficient for the transformation to occur. For martensitic transformation (6), the unknown will be the lowest cooling rate which is yet sufficient for the transformation to occur. Bainitic transformation requires determining two values restricting the area of the occurrence of it. In order to achieve this result, in equation (5) an additional constituent was introduced, and in that constituent the rate of cooling was set against the mean value of it.

$$K_f = 18.4 - 15.4\cdot C - 1.9\cdot Mn + 0.7\cdot Si - 2.5\cdot Cr - 1.5\cdot Ni - 4.8\cdot Mo + 2.4\cdot V + 1.4\cdot Cu - 0.004\cdot T_A - \sqrt[4]{v_c} \tag{3}$$

$$K_p = 12 - 1.4\cdot C - 2.3\cdot Mn - 2.3\cdot Cr - 1.4\cdot Ni - 6\cdot Mo + 3.9\cdot V - 0.002\cdot T - 1.2\cdot \sqrt[4]{v_c} \tag{4}$$

$$K_b = 1.3 - 3.7\cdot C + 0.45\cdot Mn + 0.2\cdot Cr + 0.18\cdot Ni + 1.9\cdot Mo - 0.17\cdot \sqrt[4]{v_c} - 0.57\cdot \sqrt{(4.35 - \sqrt[4]{v_c})^2} \tag{5}$$

$$K_m = -16.5 + 4.7\cdot C + 2.6\cdot Mn + 0.6\cdot Si + 2.4\cdot Cr + 1.2\cdot Ni + 1.9\cdot Mo + 4.8\cdot Cu + 0.006\cdot T_A + 1.1\cdot \sqrt[4]{v_c} \tag{6}$$

The correctness of the action of the classificators was assessed upon the basis of the coefficient of correct classifications, which was being determined as the quotient of correctly classified cases and all the examples in the data set (Table 3).

TABLE 3
Quality assessment coefficients for models, used as classifiers for determining the types of occurring transformations

| Transformation areas | Coefficient of correct classifications, % |
|---|---|
| Ferritic | 85 |
| Pearlitic | 86 |
| Bainitic | 73 |
| Martensitic | 84 |

For the hardness model, the general form of the equation was presumed (7):

$$Y = a_0 + \sum_i a_i f_i(X) \tag{7}$$

where:
Y - explained variable - hardness;
$a_0$, $a_1$ .. $a_i$ - regression coefficients;
$f_i$ – functions of equation variables;
X - vector of explanatory variables.

Into the model, it was the product of two independent variables that were introduced as well. The objective of those activities was to take under consideration the interaction between explanatory variables. The estimation of regression coefficients was performed with the application of the least squares method.

Adjusting the equation to the empirical data was assessed upon the basis of the determination coefficient $R^2$. The significance of explanatory variables added to, or removed from, the equation, was being assessed upon the basis of the values of the adjusted determination coefficient. The adjusted determination coefficient makes it possible to compare the models of multiple regression having a different number of explanatory variables, which were developed for those same empirical data. The significance of the regression coefficients of the model was researched as well verifying the hypotheses relevant to the individual coefficients of the form: the null hypothesis and the alternative hypothesis. For the verification of the hypothesis, the t-Student distribution and, determined upon the basis of it, the critical p-value of were applied. The level of significance of $\alpha$=0.05 was presumed. The statistical significance of the regression model was being researched taking advantage of the F-Fisher-Snedecor test. The models were being assessed as well upon the basis of: the mean absolute error, the standard deviation of error, and also the standard deviation quotient of the calculation error, as well as the standard deviation of the dependent variable value. The quotient of standard deviations makes it possible to set the values of the error of the model against the scope of changes in dependent variable.

The hardness of a steel cooled at a particular rate (vc) from the austenitizing temperature (TA) is described in the equation (8). In the model, there are independent variables: the mass concentrations of elements, the austenitizing temperature, the cooling rate, and also four dichotomous variables determining the kind of constituents occurring in the microstructure of a steel. In the equation, it was the interactions between the mass concentration of carbon and the cooling rate that were taken under consideration as well.

Moreover, the hardness of steel was described in addition to that with the application of two equations which may be applied for a martensitic structure (9), and also for the ferritic- pearlitic one (10). The statistics of the models, including the following values: the mean absolute error, the standard deviation of error, the quotient of standard deviations, and also the coefficient of correlation, were compiled in Tables 4 and 5.

$$HV = 3.7 + 225 \cdot C + 82 \cdot Mn + 28 \cdot Si + 55 \cdot Cr + 28 \cdot Ni + 53.5 \cdot Mo + 147 \cdot V + 71 \cdot Cu + 0.09 \cdot T_A - 3.8 \cdot \sqrt[4]{v_c} + 68 \cdot C \cdot \sqrt[4]{v_c} - 42 \cdot W_f - 69 \cdot W_p - 32.5 \cdot W_b + 72 \cdot W_m \quad (8)$$

$$HV_m = 200 + 824 \cdot C + 44 \cdot Mn + 14 \cdot Cr + 9 \cdot Ni + 171 \cdot V + 78.5 \cdot Cu + 4.13 \cdot \sqrt[4]{v_c} \quad (9)$$

$$HV_{f-p} = -73 + 253 \cdot C + 52 \cdot Mn + 10 \cdot Si + 36 \cdot Cr + 8 \cdot Ni + 20 \cdot Mo + 80 \cdot V + 0.11 \cdot T_A + 12.5 \cdot \sqrt[4]{v_c} \quad (10)$$

The hardness models for a martensitic structure, and for the ferritic- pearlitic one, may be applied after obtaining the appropriate results of classifications. In the case of uncertain results of classifications if the coefficient of Wx assumes the values similar to the threshold values dividing separate classes, it is a better solution to apply the general model.

TABLE 4
Values of statistics used to evaluate the significance of the developed models

| | Model | | |
|---|---|---|---|
| | HV | HVm | HVf-p |
| $R^2$ | 0.848 | 0.857 | 0.746 |
| Adjusted $R^2$ | 0.847 | 0.855 | 0.743 |
| Standard error | 62.3 | 39.9 | 24.4 |
| Observations | 2845 | 418 | 667 |
| Significance F | 0 | 6E-169 | 3E-189 |

TABLE 5
Values of statistics used to evaluate the quality of the developed models

| | Mean absolute error, HV | Standard deviation of the error, HV | Ratio of standard deviations | Pearson's correlation coefficient |
|---|---|---|---|---|
| HV | 48.5 | 38.9 | 0.24 | 0.92 |
| HVm | 30.5 | 25.2 | 0.24 | 0.92 |
| HVf-p | 19.4 | 14.5 | 0.30 | 0.86 |

For hardness models the following scatter plots for dependent variable values that were experimental and calculated using equations (8)-(10) were made. The results are shown in Fig. 1.

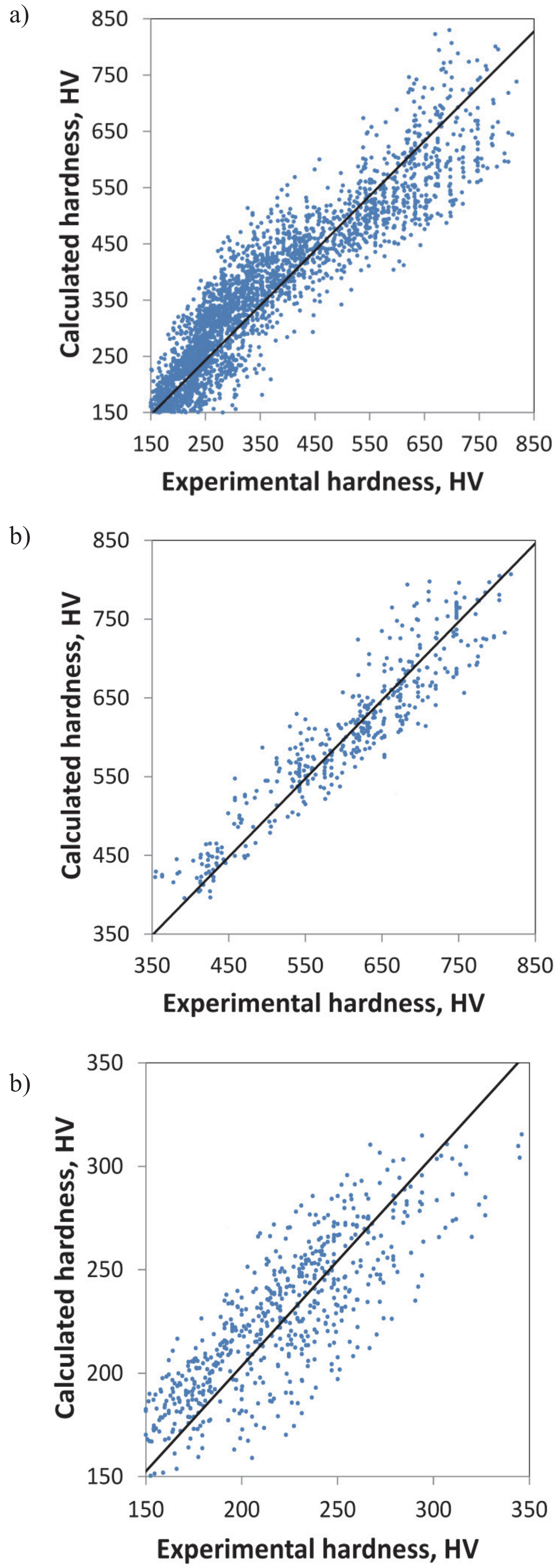


Fig. 1. Comparison of the experimental hardness (HV) with values calculated using the regression model: a) HV equation (8); b) HVm equation (9); c) HVf-p equation (10)

The hardness model was numerically verified by means of comparison between the curves of hardness determined experimentally and the calculated ones. The calculations were performed for data which were not taken advantage of for the purpose of developing the model. The verification collection was composed of 30 chemical compositions of structural steel. The examples of the results were presented in Fig. 2 and Fig. 3.

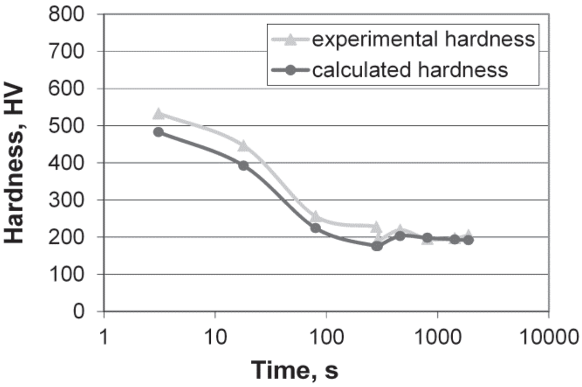


Fig. 2. Comparison of the experimental and calculated hardness curves for the steels with a mass concentration of elements: 0.23%C, 1.53%Mn, 0.4%Si, 0.03%Cr austenitised at temperature of 900°C

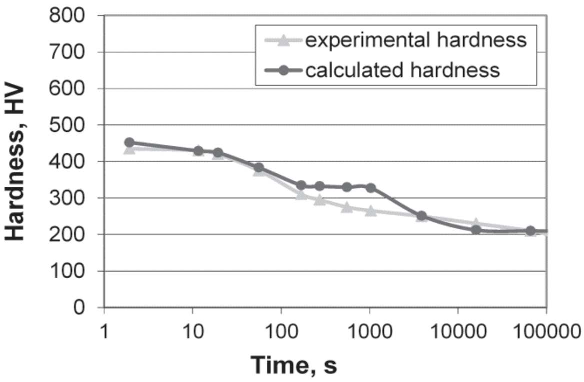


Fig. 3.Comparison of the experimental and calculated hardness curves for the steels with a mass concentration of elements: 0.13%C, 0.46%Mn, 0.26%Si, 0.78%Cr, 3,69%Ni, 0.04%Mo, 0.16%Cu austenitised at temperature of 870°C

## 4. Summary

The advantage of the multiple regression method is the fact that it is a model which is easy to be applied and to be disseminated. The results of the estimation of the hardness of steels are burdened with certain errors. Those result both from simplifications applied in the course of modelling, as well as from the specific character of empirical data upon the basis of which the model was developed. The data set was developed upon the basis of the published CCT diagrams. The CCT diagrams included in the paper were being developed for several years by different research laboratories. The error being made in the course of the analysis of chemical composition, or the measurement of hardness, was undergoing significant changes. A significant problem is constituted as well by the graphic form of data and errors connected with making CCT diagrams and printing them, and also errors resulting from the digitalization of data.

Every vector of data taken advantage of in the course of the calculations of regression coefficients has to contain the values of all variables. Information relevant to the time of austenitizing, and also to the grain size, was not being provided on the majority of the CCT diagrams, and, for that very reason, it was not taken under consideration in the model. 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 hardness model for structural steels, continuously cooled from the austenitizing temperature, was developed as well with the application of the artificial neural networks method. The verification of it is currently in progress.

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, critical temperatures of steel and volume fractions of ferrite, pearlite, bainite and martensite in the microstructure of steel. Some results are shown in papers [20-21] New models describing the transformations of supercooled austenite will be taken advantage of for the purpose of modification of a computer program [23] for the purpose of the calculations of CCT diagrams for structural steels.


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