

# Calculation of volume fractions of microstructural components in steels cooled from the austenitizing temperature

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## ABSTRACT

**Purpose:** The paper presents method in predicting the volume fractions of ferrite, pearlite, bainite and martensite of steel cooled continuously from the austenitizing temperature, basing on the chemical composition, austenitizing temperature and cooling rate.

**Design/methodology/approach:** In the paper it has been applied a hybrid approach that combined application of various mathematical tools including logistic regression and multiple regression to solve selected tasks from the area of materials science.

**Findings:** Computational methods are an alternative to experimental measurement in providing the material data required for heat treatment process simulation.

**Research limitations/implications:** All equations are limited by range of mass concentrations of elements which is presented in Table 2.

**Practical implications:** The worked out formulae may be used in computer systems of steels' designing for the heat-treated machine parts.

**Originality/value:** The paper presents the method for calculating the volume fractions of ferrite, pearlite, bainite and martensite of the structural steels, depending on their chemical composition, austenitizing temperature and cooling rate.

**Keywords:** Computational Material Science; Steels; Statistic Methods; CCT diagrams

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## ANALYSIS AND MODELLING

### 1. Introduction

Progress in the field of materials science is inextricably linked with the application and development of computational methods, numerical methods, methods of computational intelligence and artificial intelligence.

Mathematical modelling, computational intelligence and artificial intelligence indicate to the big potential connected with using this methods in the field of material engineering [1-10].

The continuous cooling transformation (CCT) diagrams describe the transformations taking place during continuous

cooling at different cooling rates from austenitizing temperature. The CCT diagrams provide information on the transformation start and finish temperatures, hardness of steel and volume fractions of microstructural constituents for each particular cooling rate.

This allows to predict the microstructure, transformations temperature and hardness of steels after heat treatment like quenching, normalizing and fully annealing. The dilatometric method supplemented with metallographic investigations with different velocities of samples and their hardness measurements are usually used for establishing a CCT diagrams. The investigations are time consuming and require costly research apparatuses. These are the main reason 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 formulae developed after many experiments [11-14].

A method of modelling CCT diagrams with the use of neural networks has been described in detail in the publications [15-18]. Another example of method application for CCT diagrams calculation is a model presented in [19] that employs multiple regression method and artificial neural networks.

The paper presents the methodology of modelling using the regression method of the relationship between the chemical composition and the volume fractions of the structural constituents of the steel cooling from the austenitizing temperature.

## 2. Materials and method

Basing on the literature information, the data set was worked out containing chemical compositions, austenitizing temperatures, as well as and volume fractions of the microstructural components as functions of the cooling rate. Data required for model development were prepared basing on the CCT diagrams. Mass concentrations of the particular alloying elements, cooling rate, and austenitising temperature were used as input data. The data set consisted of 500 CCT diagrams. The number of cases for particular data sets has been presented in Table 1. A range of the accepted mass concentrations of the elements has been presented in Table 2. Multicollinearity among the independent variables were evaluated using correlation matrix (Table 3). Estimation coefficients of the regression equation was carried out using least squares method. The assessment of the significance of the regression coefficients were made using the Student's t-test. The independent variables are statistically significant in

explaining the variation in the volume fractions of the microstructural constituents if p-values are less than 0.05 for the significance level of 5%.

Table 1.  
Number of cases in data sets

|                | Data set |          |         |            |
|----------------|----------|----------|---------|------------|
|                | Ferrite  | Pearlite | Bainite | Martensite |
| Regression     | 1586     | 1586     | 1586    | 1586       |
| Classification | 5380     | 5380     | 5380    | 3388       |

Table 2.  
Ranges of mass concentrations of elements

| Range              | Mass fractions of elements, % |      |      |      |      |      |      |      |
|--------------------|-------------------------------|------|------|------|------|------|------|------|
|                    | C                             | Mn   | Si   | Cr   | Ni   | Mo   | V    | Cu   |
| min                | 0.11                          | 0.12 | 0.1  | 0    | 0    | 0    | 0    | 0    |
| max                | 0.60                          | 2.04 | 1.7  | 2.24 | 3.85 | 1.05 | 0.46 | 0.38 |
| average            | 0.32                          | 0.77 | 0.39 | 0.84 | 0.78 | 0.17 | 0.04 | 0.08 |
| standard deviation | 0.13                          | 0.36 | 0.31 | 0.52 | 1.04 | 0.22 | 0.08 | 0.09 |

Table 3.  
Correlation matrix for independent variables

|                | C     | Mn    | Si    | Cr   | Ni    | Mo   | V     | Cu   | T <sub>A</sub> |
|----------------|-------|-------|-------|------|-------|------|-------|------|----------------|
| C              | 1     |       |       |      |       |      |       |      |                |
| Mn             | 0.09  | 1     |       |      |       |      |       |      |                |
| Si             | 0.17  | -0.02 | 1     |      |       |      |       |      |                |
| Cr             | 0.02  | -0.40 | -0.20 | 1    |       |      |       |      |                |
| Ni             | -0.24 | -0.38 | -0.21 | 0.18 | 1     |      |       |      |                |
| Mo             | -0.18 | -0.25 | -0.10 | 0.19 | 0.20  | 1    |       |      |                |
| V              | 0.13  | -0.02 | 0.13  | 0.23 | -0.15 | 0.36 | 1     |      |                |
| Cu             | 0.08  | -0.19 | -0.08 | 0.12 | 0.01  | 0.11 | -0.01 | 1    |                |
| T <sub>A</sub> | -0.08 | -0.04 | 0.15  | 0.07 | -0.28 | 0.14 | 0.30  | 0.03 | 1              |

On the basis of the analysis of different forms, general formula embracing the influence of the chemical composition and austenitizing temperature as well as cooling rate on the volume fractions of ferrite ( $U_f$ ), pearlite ( $U_p$ ), bainite ( $U_b$ ) and martensite ( $U_m$ ), including the two way interactions between independent variables, general forms of equations have been accepted:

- for defining the volume fractions of ferrite:

$$U_f = a_0 + a_1 \cdot C + a_2 \cdot Mn + a_3 \cdot Si + a_4 \cdot Cr + a_5 \cdot Ni + a_6 \cdot Mo + a_7 \cdot T_A + a_8 \cdot v_c^{0.25} + a_9 \cdot C \cdot v_c^{0.25} + a_{10} \cdot W_f + a_{11} \cdot W_p + a_{12} \cdot W_b + a_{13} \cdot W_m \quad (1)$$

- for defining the volume fractions of pearlite:

$$U_p = a_0 + a_1 \cdot C + a_2 \cdot Mn + a_3 \cdot Si + a_4 \cdot Cr + a_5 \cdot Mo + a_6 \cdot v_c^{0.25} + a_7 \cdot C \cdot v_c^{0.25} + a_8 \cdot W_f + a_9 \cdot W_p + a_{10} \cdot W_b + a_{11} \cdot W_m \quad (2)$$

- for defining the volume fractions of bainite:

$$U_b = a_0 + a_1 \cdot C + a_2 \cdot Mn + a_3 \cdot Si + a_4 \cdot Mo + a_5 \cdot Cu + a_6 \cdot T_A + a_7 \cdot C \cdot v_c^{0.25} + a_8 \cdot W_f + a_9 \cdot W_p + a_{10} \cdot W_b + a_{11} \cdot W_m \quad (3)$$

- for defining the volume fractions of martensite:

$$U_m = a_0 + a_1 \cdot C + a_2 \cdot Mn + a_3 \cdot Si + a_4 \cdot Cr + a_5 \cdot Ni + a_6 \cdot Mo + a_7 \cdot Cu + a_8 \cdot T_A + a_9 \cdot v_c^{0.25} + a_{10} \cdot C \cdot v_c^{0.25} + a_{11} \cdot W_f + a_{12} \cdot W_p + a_{13} \cdot W_b + a_{14} \cdot W_m \quad (4)$$

where:

C, Mn, Cr, Ni, Mo, V – mass fractions of the alloying elements;

$a_0, a_1, \dots, a_{14}$  – coefficients calculated with the regression analysis;

$T_A$  – austenitizing temperature, °C;

$v_c$  – cooling rate, °/min.

$W_f, W_p, W_b, W_m$  – dichotomous variables, whose values (0 or 1) were determined basing on the binomial logistic regression model.

The type of microstructure developed after cooling the steel was specified using four binary nominal variables, whose values were determined basing on the logistic regression model. A classifier had to be developed, to obtain this information, using as input data the mass concentrations of the elements, austenitizing temperature, and cooling rate. The particular classifiers were developed using logistic regression. The general form of formulae are presented in equations (5)-(6). The assessment of the significance of the regression coefficients were made using the Wald chi-square test.

$$W_X = \exp(S_X) / \{1 + \exp(S_X)\} \quad (5)$$

where:

$X = f$  (ferrite),  $p$  (pearlite),  $b$  (bainite),  $m$  (martensite),

$$S_X = b_{0X} + b_{1X} \cdot C + b_{2X} \cdot Mn + b_{3X} \cdot Cr + b_{4X} \cdot Ni + b_{5X} \cdot Mo + b_{6X} \cdot V + b_{7X} \cdot T_A + b_{8X} \cdot v_c \quad (6)$$

### 3. Calculation results

The formulae describing the influence of the chemical composition and cooling rate on the volume fractions of the microstructural constituents worked out using the multiple regression, are presented in equations (7)-(14). Classifiers used for forecasting occurrences of the particular microstructural constituents in steel are presented in equations (5)-(6), (15)-(18). Example of the assessment of the significance of the regression coefficients for volume fraction of ferrite are presented in Table 4.

Table 4.

The assessment of significance of regression coefficients

|                      | Coefficients | Standard Error | t Stat   | P-value  |
|----------------------|--------------|----------------|----------|----------|
| Intercept            | 116.0372     | 6.313174       | 18.38016 | 1.71E-68 |
| C                    | -132.742     | 5.615895       | -23.6369 | 6.2E-106 |
| Mn                   | -9.51104     | 1.246579       | -7.62971 | 4.05E-14 |
| Si                   | -3.02052     | 1.275324       | -2.36843 | 0.017984 |
| Cr                   | -9.90187     | 0.871307       | -11.3644 | 8.11E-29 |
| Ni                   | -4.99392     | 0.481712       | -10.367  | 2.1E-24  |
| Mo                   | -4.02409     | 1.839577       | -2.18751 | 0.028852 |
| $T_A$                | -0.02137     | 0.005449       | -3.92227 | 9.15E-05 |
| $v_c^{0.25}$         | -6.16667     | 0.416565       | -14.8036 | 1.62E-46 |
| $C \cdot v_c^{0.25}$ | 12.25599     | 1.20891        | 10.13805 | 1.94E-23 |
| $W_f$                | 10.16293     | 1.125498       | 9.029713 | 4.91E-19 |
| $W_p$                | 5.799526     | 1.18136        | 4.909195 | 1.01E-06 |
| $W_b$                | -9.30904     | 0.891163       | -10.4459 | 9.68E-25 |
| $W_m$                | -11.0791     | 1.213641       | -9.12883 | 2.07E-19 |

$$F(\%) = \begin{cases} 0 & \text{for } W_f = 0 \\ 0 & \text{for } U_f \leq 0 \\ U_f & \text{for } U_f > 0 \end{cases} \quad (7)$$

$$U_f = 116 - 132.7 \cdot C - 9.5 \cdot Mn - 3 \cdot Si - 10 \cdot Cr - 5 \cdot Ni - 4 \cdot Mo - 0.021 \cdot T_A - 6.17 \cdot v_c^{0.25} + 12.2 \cdot C \cdot v_c^{0.25} + 10.2 \cdot W_f + 5.8 \cdot W_p - 9.3 \cdot W_b - 11.1 \cdot W_m \quad (8)$$

$$P(\%) = \begin{cases} 0 & \text{for } W_p = 0 \\ 0 & \text{for } U_p \leq 0 \\ U_p & \text{for } U_p > 0 \end{cases} \quad (9)$$

$$U_p = -5.2 + 98.2 \cdot C + 3.1 \cdot Mn + 6.5 \cdot Si + 3 \cdot Cr - 8.2 \cdot Mo + 3.7 \cdot v_c^{0.25} - 15.3 \cdot C \cdot v_c^{0.25} - 5.1 \cdot W_f + 25.2 \cdot W_p - 11 \cdot W_b - 18.2 \cdot W_m \quad (10)$$

$$B(\%) = \begin{cases} 0 & \text{for } W_b = 0 \\ 0 & \text{for } U_b \leq 0 \\ U_b & \text{for } U_b > 0 \end{cases} \quad (11)$$

$$U_b = -11.5 + 25.8 \cdot C - 7.4 \cdot Mn - 7.2 \cdot Si + 4.6 \cdot Mo - 20.8 \cdot Cu + 0.03 \cdot T_A - 9.1 \cdot C \cdot v_c^{0.25} + 13.1 \cdot W_f - 18.4 \cdot W_p + 34.8 \cdot W_b + 6.2 \cdot W_m \quad (12)$$

$$M(\%) = \begin{cases} 0 & \text{for } W_m = 0 \\ 0 & \text{for } U_m \leq 0 \\ U_m & \text{for } U_m > 0 \end{cases} \quad (13)$$

$$U_m = 10.2 + 2.8 \cdot C + 13.7 \cdot Mn + 4.2 \cdot Si + 7.8 \cdot Cr + 4.9 \cdot Ni + 8.1 \cdot Mo + 14.5 \cdot Cu - 0.02 \cdot T_A + 2 \cdot v_c^{0.25} + 13.7 \cdot C \cdot v_c^{0.25} - 18.2 \cdot W_f - 12.1 \cdot W_p - 14.3 \cdot W_b + 23.2 \cdot W_m \quad (14)$$

The values of the coefficients:  $W_f$ ,  $W_p$ ,  $W_b$ ,  $W_m$  would be calculated using equations (5)-(6) and (15)-(18). Calculated using the equations (8)-(19) values of the volume fractions of microstructure components were scaled proportionally so that their sum is equal to 100.

$$K_f = 18.4 - 15.4 \cdot C - 1.9 \cdot Mn + 0.7 \cdot Si - 2.5 \cdot Cr - 1.5 \cdot Ni - 4.8 \cdot Mo + 2.4 \cdot V + 1.4 \cdot Cu - 0.004 \cdot T_A \cdot v_c^{0.25} \quad (15)$$

$$K_p = 12 - 1.4 \cdot C - 2.3 \cdot Mn - 2.3 \cdot Cr - 1.4 \cdot Ni - 6 \cdot Mo + 3.9 \cdot V - 0.002 \cdot T_A - 1.2 \cdot v_c^{0.25} \quad (16)$$

$$K_b = 1.3 - 3.7 \cdot C + 0.45 \cdot Mn + 0.2 \cdot Cr + 0.18 \cdot Ni + 1.9 \cdot Mo - 0.17 \cdot v_c^{0.25} - 0.57 \cdot [(4.35 - v_c^{0.25})^2]^{0.5} \quad (17)$$

$$K_m = -16.5 + 4.7 \cdot C + 2.6 \cdot Mn + 0.6 \cdot Si + 2.4 \cdot Cr + 1.2 \cdot Ni + 1.9 \cdot Mo + 4.8 \cdot Cu + 0.006 \cdot T_A + 1.1 \cdot v_c^{0.25} \quad (18)$$

The quality assessment coefficients of the classifier are presented in Table 5. The lowest mean error value was obtained by using formula describing the influence of chemical composition, austenitizing temperature and cooling rate on the volume fraction of ferrite. The highest mean error value was obtained for model describing volume fraction of bainite. Mean error values, standard deviation of the error and the correlation coefficient for the volume fractions of ferrite, pearlite, bainite and martensite are given in Table 6.

Table 5.

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  |

To verify the model worked out, the experimental volume fractions of ferrite, pearlite, bainite and martensite curves were compared with curves calculated using the empirical formulae. Examples of the diagrams worked out are shown in Figs. 1-4.

An example of the comparative diagrams showing changes of volume fractions of the microstructural constituents depending on time required to cooling the steel from the austenitizing temperature for results obtained using the empirical formulae and the experimental data are shown in Figs. 5-7.

Table 6.

Error values and correlation coefficients for volume fraction of microstructural constituent model

| Microstructural constituent | Mean absolute error, % | Standard deviation of the error, % | Quotient of standard deviations | Pearson correlation coefficient |
|-----------------------------|------------------------|------------------------------------|---------------------------------|---------------------------------|
| Ferrite                     | 9.5                    | 9.7                                | 0.37                            | 0.87                            |
| Pearlite                    | 9.9                    | 11.3                               | 0.39                            | 0.86                            |
| Bainite                     | 15.8                   | 14.2                               | 0.44                            | 0.76                            |
| Martensite                  | 12.3                   | 12.6                               | 0.31                            | 0.91                            |

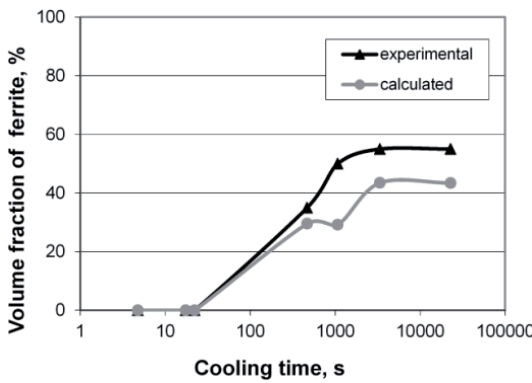


Fig. 1. The comparison of the experimental and calculated volume fractions of ferrite for the steels with a mass concentration of elements 0.38%C, 0.74%Mn, 0.26%Si, 0.9%Cr, 0.26%Ni, 0.17%Cu austenitised at temperature of 880°C

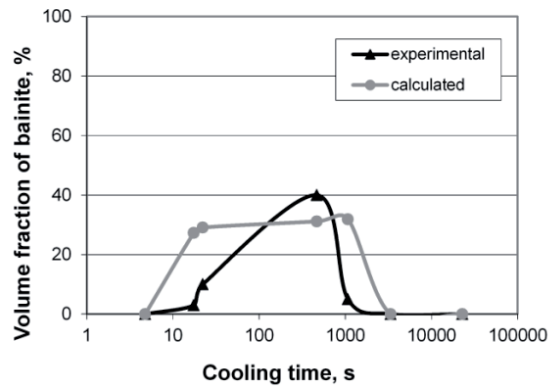


Fig. 3. The comparison of the experimental and calculated volume fractions of bainite for the steels with a mass concentration of elements 0.38%C, 0.74%Mn, 0.26%Si, 0.9%Cr, 0.26%Ni, 0.17%Cu austenitised at temperature of 880°C

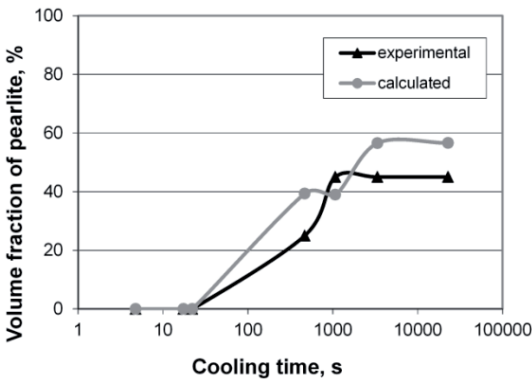


Fig. 2. The comparison of the experimental and calculated volume fractions of pearlite for the steels with a mass concentration of elements 0.38%C, 0.74%Mn, 0.26%Si, 0.9%Cr, 0.26%Ni, 0.17%Cu austenitised at temperature of 880°C

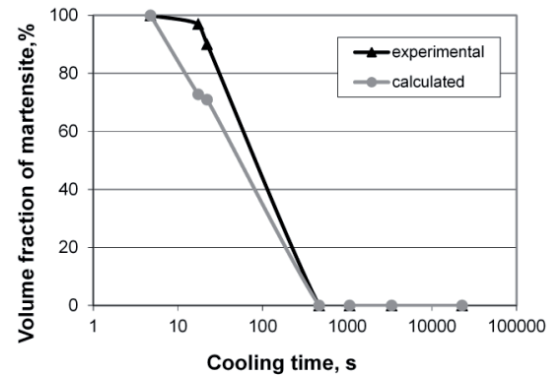


Fig. 4. The comparison of the experimental and calculated volume fractions of martensite for the steels with a mass concentration of elements 0.38%C, 0.74%Mn, 0.26%Si, 0.9%Cr, 0.26%Ni, 0.17%Cu austenitised at temperature of 880°C

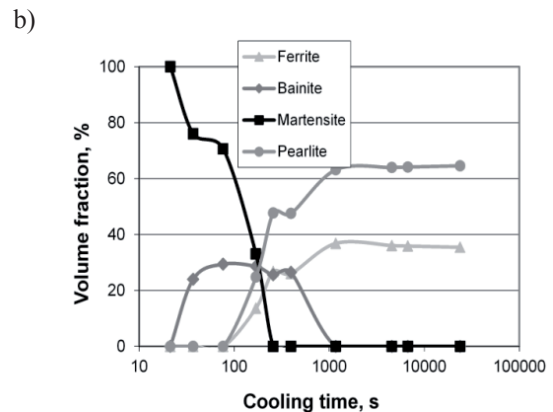
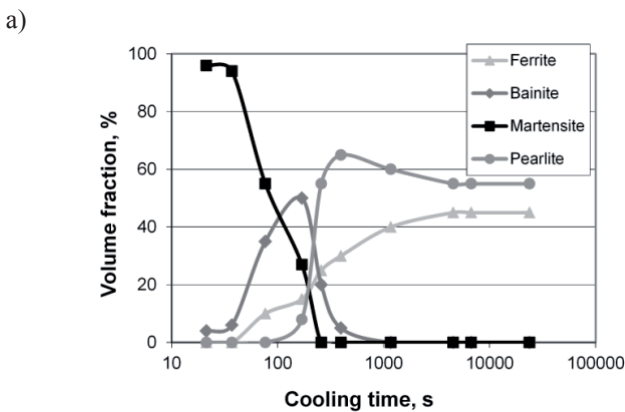


Fig. 5. Fractions of the microstructural constituents in steel with concentrations of: 0.47% C, 1.37% Mn, 0.36% Si, 0.15%Cr, 0.19%Cu, austenitized at temperature of 875°C, a) experimental, b) calculated

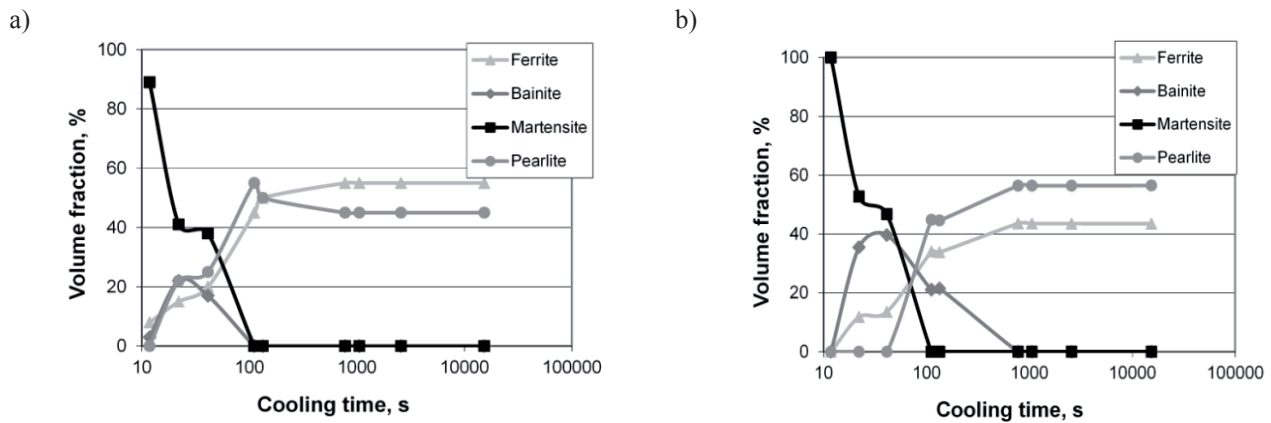


Fig. 6. Fractions of the microstructural constituents in steel with concentrations of: 0.38% C, 0.79% Mn, 1.37% Si, 0.15%Cr, 0.16%Ni, austenitized at temperature of 880°C, a) experimental, b) calculated

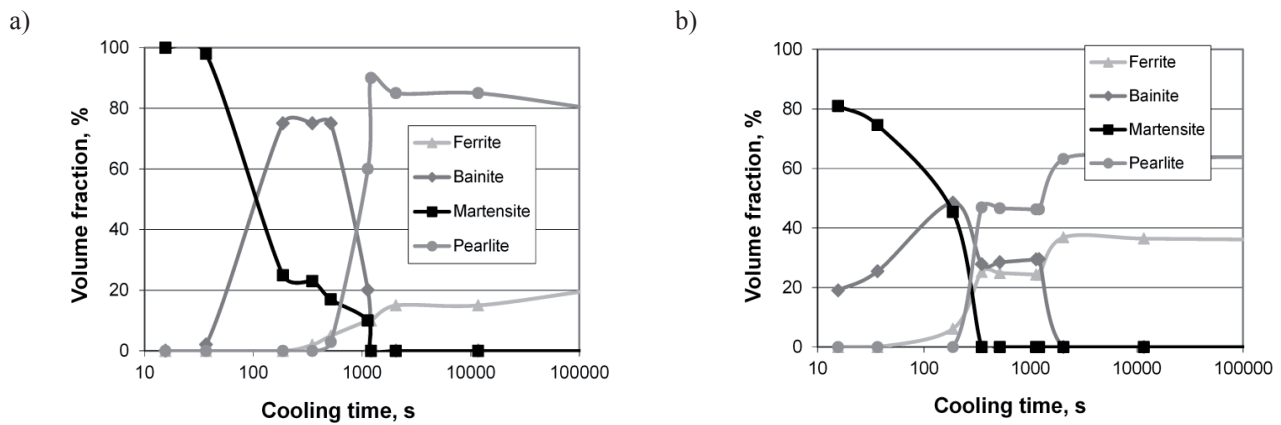


Fig. 7. Fractions of the microstructural constituents in steel with concentrations of: 0.43% C, 1.67% Mn, 0.28% Si, 0.32%Cr, 0.11%Ni, 0.1%V, austenitized at temperature of 870°C, a) experimental, b) calculated

## 4. Summary

Multiple regression and logistic regression were used to develop formulae for calculating volume fractions of ferrite, pearlite, bainite and martensite. The model worked out makes it possible to calculate volume fractions of the microstructural constituents for the steel with a known chemical composition. Determining the volume fractions of the microstructural constituents, according to the method proposed in this paper, calls for determining the types of the microstructure that occur in the steel after cooling from the austenitising temperature. The types of the microstructural constituents were determined using four dichotomous variables containing the information if the following constituents are present in the structure: ferrite,

pearlite, bainite, martensite. A classifier had to be developed, to obtain this information, using as input data chemical composition cooling rate and austenitising temperature. In this work, the austenite grain size and austenitizing time, have not been taken into account because of the lack of the information in the majority of CCT diagrams used for preparing the data set.

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