A NUMERICAL SIMULATION OF STEEL QUENCHING

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Abstract
This article deals with the appropriate setting of marginal conditions for the creation of mathematical model. For description of transformation kinetics of diffusion Johnson-Mehl-Avrami-Kolmogorov equation was utilized and for the construction of FEM model the pattern Ø25mm x 50 mm was used. Determined FEM model was verified experimentally and results showed that there is good agreement between the mathematical model and the experimental method. From conducted study it follows that FEM models can be utilized for the design and optimization of thermal processing and that these models are important tools for heat treatment prediction.

Key words: FEM model, microstructure, steels.

INTRODUCTION

Mathematical models are important for the design and optimization of heat treatment. Their application in the production enables prediction of microstructure. Mathematical models require low time consumption and finances sources than practical tests. Compilation of mathematical models requires knowledge of several important parameters such as: physical parameters of the material, the chemical composition of the material, boundary conditions of the material (heat capacity, thermal conductivity, density, temperature of phase transformation) (SERAJZADEH, 2004; ŞIMŞIR A GÜR, 2008). Another important condition is the knowledge of heat flux during cooling. Heat flux is usually calculated based on experimental measurements (PRABHU A PRASAD 2003; BARDELCIK ET AL., 2014) however it can be also modelled, but this solution requires a very demanding model on discretization and complicated and time-consuming calculation (DU ET AL., 2016; CARON ET AL., 2013).

Quenching parameters such as heating temperature, the type of cooling medium influencing the phase transformation from austenite to bainite, pearlite, ferrite and martensite in dependence on the chemical composition of the material (YU ET AL., 2010; YANG ABHADESHIA, 2009). Obviously it is very well known that these quenching parameters can be optimized using mathematical models. Isothermal cooling models are formed with Johnson-Mehl-Avrami-Kolgomov equations for diffusion transformation. These equations are a function of nucleation and growth of a new phase from austenite in dependence on time (KIANEZHAD A SAJJADI, 2013; NEUMANN A BÖHLKE, 2016). For a non-diffusion transformation are used Koistinen-Marburger equations where transformation from austenite to martensite is a function of temperature (NEUMANN A BÖHLKE, 2016; CASEIRO ET AL., 2011). Time of the beginning and time of the end of phase transformations are other important boundary conditions which should also be considered in development of mathematical model. These data are determined from the CCT diagrams for the steel (BABU A PRASANNA KUMAR, 2014; KIM ET AL., 2007; YUAN ET AL., 2003).

The aim of this article is to propose a system for calculating and to determine algorithms which will calculate and predict the microstructure of carbon steels during their heat treatment in various cooling environments.

MATERIALS AND METHODS

The Neumann's boundary conditions together with Lagrange algorithm were chosen to complete the FEM model (DOMAŃSKI A BOKOTA, 2011; PIEKARSKA ET AL., 2011).

In this model the heat flux was used as one of the Neumann's boundary conditions. Practical experiment to determine heat flux was measured on the cylinder ø25-50 mm made of steel 25CrMo4. Heat treatment was carried out at temperatures of heating of 800°C, 900°C and 1000°C. Water was chosen as the cooling medium for the quenching. Temperatures were recorded during the heat treatment in the axis and on the surface of the cylinder. Measured data (temperatures depending on time) was processed in the program Scilab 5.5.1. (SCILAB ENTERPRISES, 2014) in which the algorithms were solute. Heat flux was calculated from

the data for hardening (LI A WELLS, 2005; FERNANDES A PRABHU, 2007).
Specific heat capacity *cp* and coefficient of thermal conductivity λ were other boundary conditions which were taken from published data (HUO ET AL., 2015).
Next step for the assembly FEM model was to create mesh. The density of the mesh was chosen based on the sample size (ø25-50 mm). Mesh had the highest density on the surface; toward to the middle of the cylinder the mesh was less dense. Condition that the calculation must not diverge was met. The calculation was terminated using an algorithm and mesh density was not changed by the algorithm. A model describing the temperature field counting on nontransient heat conduction was described by equation 1:

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+Q=\rho\times c\times\frac{\partial \mathrm{T}}{\partial \mathrm{t}} \quad (1)$$

Where: k – thermal conductivity (W×m^{-1}×K^{-1}), Q – inner heat – generation rate per unit volume (J× m^{-3}), T – temperature (K), q – heat transfer coefficient (W×m^{-2}×K^{-1}), ρ – density (kg×m^{-3}), c – heat capacity (J×kg^{-1}×K^{-1}), t – time (s).

Heat capacity and heat thermal coefficient were determined by iteration algorithm from measured data.
Phase transformation from austenite to martensite is nondiffusion process. Koistinen-Hamburger Displacive law describes the process as a function of temperature - Equation 2, 3.

$$\mathrm{V_m}=1-e^{-\alpha\times(Ms-T)} \quad (2)$$

$$\mathrm{V_{P,B}}=1-e^{-k\times t^n} \quad (3)$$

Where: *α, Ms* – constants based on material type (-), *k* – constant dependent on temperature (-), *n* – Avrami's exponent (-)

Phase transformations from austenite to ferrite, perlite or bainite are diffusion processes that are time dependent. The kinetics of diffusion transformation was described by Johnson-Mehl-Avrami-Kolmogorov equation. Approximate solution of development phases of the individual transformations was predicted on the basis of data from TTT diagram (CHOTĚBORSKÝ AND LINDA, 2015; SINHA ET AL., 2007). The algorithm for the calculation was written in Basic (MICROSOFT, 2010) because processed data were filed faster by visual basic than by already mentioned Scilab(SCILAB ENTERPRISES, 2014).
Derivation of equations 2 and 3 were performed to determine the amount of emerging new phase. Speed generated phase per unit of time was thereby obtained. So obtained equations were modified for the numerical solution (4-6).

$$\mathrm{Vf}=\sum_{i=1}^{n}-Kf\times Nf\times t^{Nf-1}\times e^{-Kf\times t^{Nf}}\times(1-Vf_{\max}) \quad (4)$$

$$\mathrm{Vp}=\sum_{i=1}^{n}-Kp\times Np\times t^{Np-1}\times e^{-Kp\times t^{Np}}\times(1-Vf) \quad (5)$$

$$\mathrm{Vb}=\sum_{i=1}^{n}-Kb\times Nb\times t^{Nb-1}\times e^{-Kb\times t^{Nb}}\times(1-Vf-Vp) \quad (6)$$

Where: *Vf* – volume of ferite phase (-), *Vp* – volume of pearlite phase (-), *Vb* – volume of bainite phase (-), *Kf, Kp, Kb* – overall rate constant of feritic, pearlitic and bainitic transformation that generally depends on temperature (-), *Nf, Np, Nb* – Avrami's exponent for feritic, pearlitic and bainitic transformation that depends on temperature (-).

Metallographic samples of tested steel were cut and polished from heat treated samples and etched in a solution obtained by dissolving nitric acid (2 ml) in ethanol (100 ml) Nital. The nital etchant was used for the determination of bainite volume. Austenite phase was determined by using Klemm etchant (2 g K2S2O5 + 100 ml supersaturated K2S2O3 in water) where austenite phase was not attached and bainite or martensite showed dark blue colour. Phase percentage in each sample was measured using SciLab Image and Video Processing toolbox, where threshold was obtained by a binary matrix algorithm. The algorithm was written for a proportion phase's evaluation.
Correlations and index of determination were calculated between measured data and computed data.

RESULTS AND DISCUSSION

Examples of coefficients c_o, c_1 and c_2 of heat flux are shown in Equations 7-10. These coefficients determine the character of the heat flux curve depending on the relative surface temperature. The coefficients are valid for the range of heating temperatures from 800°C to 1000°C and for the temperature of cooling in the water. General equation was obtained from the individual results of experimental measurement of steel.

$$\mathrm{q(T)}=\mathrm{C_0}\times\mathrm{T}^{\mathrm{C_1}}\times(1-\mathrm{T})^{\mathrm{C_2}} \quad (7)$$

$$\mathrm{C_0}=1{,}545\mathrm{x}10-7\cdot\log(\mathrm{T})+1{,}273\cdot 108 \quad (8)$$

$$\mathrm{C_1}=-0.357\cdot\log(\mathrm{T})+3.566 \quad (9)$$

$$\mathrm{C_2}=-0.902\cdot\log(\mathrm{T})+7.299 \quad (10)$$

Where: q – heat flux (W×m^{-2}), T – relative temperature (0 to 1) calculated from *Tp* a *Ts*(-), c_o – constant

of reinforcement (-), c_1, c_2 – constant slope from the peak, may characterize curve slope (-), Tp – furnace temperature (K)

Maximum volume fraction V are already known from preliminary isothermal investigations, temperature-dependend parameters K(T) and n(T) can be determined from the measured isothermal transformation diagrams. Generally, times t_s and t_f characterizing the start and finish of isothermal austenite transformation as a function of temperature are plotted in a form C-curves in IT diagrams. According to the traditional definition of C-curves, times t_s and t_f denote 1% and 99% of relative transformed fractions, respectively. Based on the use of Eq. 3, the following relationships can be derived:

$$ln\frac{1}{1-0.01} = K \times t_s^n \quad (11)$$

and

$$ln\frac{1}{1-0.99} = K \times t_f^n \quad (12)$$

The parameters K and n can be obtained directly from Eq. 11 and 12:

$$n(T) = \frac{6.1273}{ln\frac{t_f}{t_s}} \quad (13)$$

and

$$K(T) = \frac{0.01005}{t_s^{n(T)}} \quad (14)$$

For every constant temperature it follows from consideration above, that the multi-phase model can be applied to the prediction of isothermal as well as to the anisothermal transformation processes. The pseudo-autonomous differential equation can be solved only by numerical methods, provided that model parameters V, K and n are previously estimated, and given as a function of temperature.

Data for model of phase transformation were:

Steel 51CrV4

A1=732 °C, A3=775 °C, Ms=286 °C, M50=250 °C, Bs=500 °C and limits for austenite phase transformation were:

Ferite:

Temperature range from 550 to 732 °C

$$n(T) = 39{,}714 + 0{,}13596 \times T - 0{,}000\,1098 \times T^2$$

$$K(T) = -1{,}3873 \times 10^{-3} + 1{,}19388 \times 10^{-5} \times T - 4{,}0959 \times 10^{-8} \times T^2 + 7{,}0035 \times 10^{-11} \times T^3 - 5{,}9687 \times 10^{-14} \times T^4 + 2{,}028 \times 10^{-17} \times T^5$$

Pearlite:

Temperature range from 500 to 700 °C

$$n(T) = 91{,}6391 + 0{,}512 \times T + 0{,}000\,9503 \times T^2 - 0{,}000\,000\,57653 \times T^3$$

$$K(T) = -4{,}6049 \times 10^{-4} + 4{,}124 \times 10^{-6} \times T - 1{,}47412 \times 10^{-8} \times T^2 + 2{,}62946 \times 10^{-11} \times T^3 - 2{,}34169 \times 10^{-14} \times T^4 + 8{,}3313 \times 10^{-18} \times T^5$$

Bainite:

Temperature range from 286 °C to 500 °C

$$n(T) = -0{,}4241 - 0{,}011\,852 \times T + 0{,}000\,0179\,4 \times T^2$$

$$K(T) = -1{,}004 \times 10^{-4} + 1{,}1117 \times 10^{-6} \times T - 3{,}90286 \times 10^{-9} \times T^2 + 4{,}49955 \times 10^{-12} \times T^3$$

Martensite:

Temperature range from under 286 °C

$$M(T) = 1 - e^{-0{,}01964 \times (Ms - T)}$$

Specific heat capacity and thermal conductivity are not constant during the cooling of the material such as evident from Fig. 1. It is clear that the right graph presents the dependency between thermal conductivity and a relative temperature and left graph presents dependency between the heat capacity and relative temperatures for material C60. These characteristics were determined using iteration algorithm with aid of obtained data from measurement of temperature during cooling. Each of iteration found minimal deviation between measured cooling curve and modelled temperature by FEM where dependency of thermal conductivity and thermal heat specific were fitted by Newton polygons. In the case where the deviation between measured data and predicted were minimal the algorithm began to calculate new FEM model using obtained data and boundary conditions.

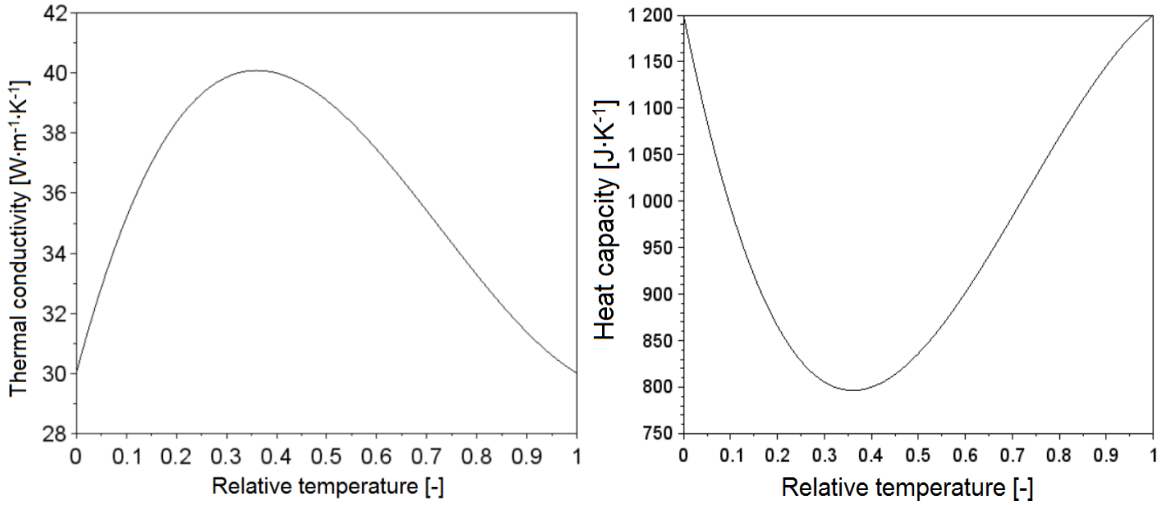

Fig. 1. – On the left side it is relationship between thermal conductivity and relative temperature and right side is relationship between heat capacity and relative temperature for material C60 – heating temperature 800°C and cooling in calm water

Content of phases depending on the distance from the surface are compared to material C60 and they are shown in Fig. 2. The sample was heated at a heating temperature of 900 °C and quenched in a calm water of 20 °C. Result shown a good correlation between predicted and measured microstructure of tested steel which was quenched in water. Correlation analysis and F-test are shown a significant dependency between computed and measured martensite volume phase (R=0.899 and F=0.9265, F_{krit}=0.4285), also for pearlite (R=0.8975 and F=1.0840, F_{krit}=2.3335), but correlation between computed and measured ferritic volume phase was not significant (R=0.6646 and F=1.6939, F_{krit}=0.4285). The computed volume phase of ferrite depend on strict boundary condition of the numerical model and each of deviance of the temperature-time kinetics dependency influence a coefficients n and k for JMAK equation. Also kinetic of austenite phase transformation of tested steel and other materials properties such as austenite grain size directly influence start and finish of transformation phase (BHADESHIA, 2004; PRABHU A FERNANDES, 2007).

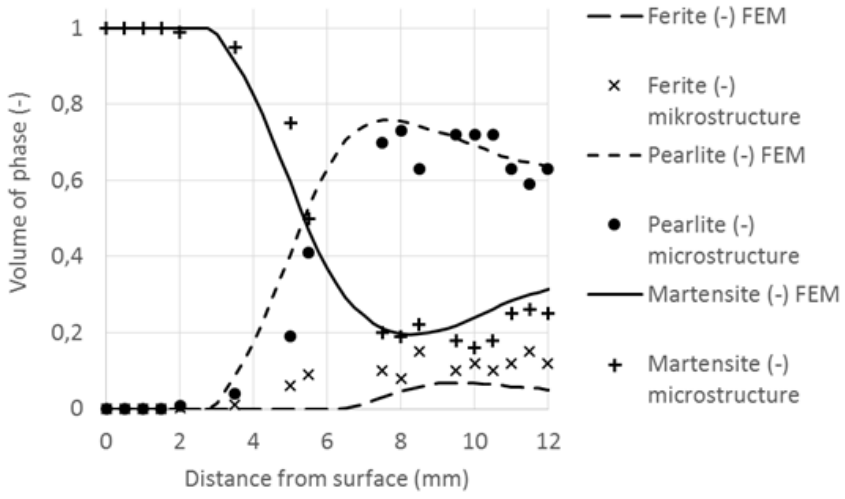

Fig. 2. – Volume of phase content depends on distance from surface

In already published study (PRASANNA KUMAR, 2013) the heat flux of different types of steel was described. It was discovered that the chemical composition of the steel significantly affects the heat flow that is one of the important boundary conditions.

The differences between the estimated phase of the model (FEM) and the experimentally determined structure were detected. These differences are caused by negligence of phase transformations, different chemical composition of the material and the grain

size. These differences can incorporate into the model. MI ET AL. (2014) also included these differences in their models of phase transformation. Differences between the model and the practical measurements have diminished, but not completely eliminated.

SERAJZADEH (2004) in his work explored the transformation of austenite phase and his results also show good agreement of FEM model and experimentally obtained data, however, they are still noticeable differences.

CONCLUSIONS

FEM model was developed to simulate thermal processing. FEM model was validated by an experimental method. The obtained results and the literature cited include the following conclusions:

- Between the model and calculations are differences. Their size may be regarded as unacceptable. Measured and calculated phase in the steel shown a good correlation
- Using the FEM model it can be predicted other properties for heat treatment such as the microstructure of the treated material.
- Described procedure can be used for an optimization of heat treatment plain carbon and low alloying steels for agriculture tools and assemblies.

This procedure can also be used to optimize the design steps of heat treatment in workshops, to set up heat treatment and their next qualitative controls.

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