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Computer simulation of microstructure of quenched moulding die

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ABSTRACT

Purpose: The research purpose is to upgrade the mathematical modelling and computer simulation of quenching of steel.

Design/methodology/approach: The computer simulation of steel hardening is consisted of numerical calculation of transient temperature field in process of cooling, and of numerical calculation of mechanical properties. The hardness has been predicted by the conversion of calculated time of cooling from 800 to 500°C at specimen points to the hardness. The algorithm is completed to solve 3-D situation problems such as the quenching of complex cylinders, cones, spheres, etc.

Findings: On the basis of control volume method, the algorithm for prediction of mechanical properties and microstructure distribution in quenched steel specimens with complex geometries has been developed. The established relations were applied in computer simulation of mechanical properties and microstructure distribution of forged steel centrifugal casting pipe mould. The investigated model of steel quenching can be successfully applied in the practice of heat treatment.

Research limitations/implications: The investigation was done on carbon and low alloyed steel. The further experimental investigations are needed for final verification of established model.

Practical implications: The established algorithms can be used in heat treating practice.

Originality/value: Microstructure distribution is estimated based on time relevant for structure transformation, i.e., the cooling time from 800 to 500°C, $t_{8/5}$.

Keywords: Quenching; Tempering; Mathematical modelling; Computer simulation; Hardness

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

The numerical simulation of mechanical properties distribution in quenched steel specimen has one of the highest priorities in simulation of phenomena of steel quenching [1-10]. During the quenching of steel many different physical processes, as are, phase transformation, evolution of microstructure, diffusion, heat conduction, and mechanical stressing and distortion are at once taken place inside metal. Despite very useful software which can be used for computer simulation of quenching, there are still questions on which answers should be given to satisfy all industry needs in mathematical modelling and simulation of steel quenching [11,12].

Simulation of heat transfer is thermodynamical problem. There is necessary to establish the appropriate algorithm which describes cooling process, and to involve appropriate input data in model. The accuracy of numerical simulation of thermal process directly depends on the applied input data. Inverse heat transfer problems should be solute to determine heat transfer coefficients for quenching based on experimentally evaluated cooling curve results [12]. Using of experimentally predicted heat transfer coefficient is possible only if all of heat transfer parameters are same in simulated process of quenching as was in experimental evaluation of the heat transfer coefficient [12]. Except heat transfer coefficient a heat conductivity, heat capacity and other relevant material properties should be estimated. It can be done by calibrating of all input data according to the Crafts-Lamont diagrams [13].

Usually simulations of microstructural transformations are based on the both, CCT diagrams using linear alignment with the actual chemical composition, or on the thermo-kinetic expressions [12]. The first approach is more consistent, but generally does not give accurate results. Hardness and microstructure distribution in quenched specimen can be found out based on characteristic cooling time relevant for microstructure transformation. It can be accepted that if the cooling time from 800 to 500°C, $t_{8/5}$, is equal for two different specimens of same kind of steel the hardness and microstructure composition of these two specimens should be equal to each other [14].

2. Computer modelling of heat transfer

Modelling and computer simulation of heat transfer is in the root of all modelling and computer simulation of quenching. Thermal process usually should be considered with a transient temperature field. The transient temperature field in an isotropic rigid body is described by Fourier's law of heat conduction:

$$\frac{\delta(c\rho T)}{\delta t} = div\lambda\, gradT \tag{1}$$

where λ/Wm^{-1}K^{-1} is coefficient of heat conductivity, ρ/kgm^{-3} is density, and c/Jkg^{-1}K^{-1} is specific heat capacity. Characteristic boundary condition is:

$$-\lambda \frac{\delta T}{\delta n}\bigg|_{s} = \alpha\left(T_s - T_f\right) \tag{2}$$

where T_s/K is surface temperature, T_f/K is quenchant temperature, α/Wm^{-2}K^{-1} is heat transfer coefficient.

Solution of equation (1) can be found out using the finite volume method [15, 16]. Discretization system has N linear algebraic equations with N unknown temperatures of control volumes, where N is total number of control volumes. Time of cooling from T_a to specific temperature in particular point is determined as sum of time steps, and in this way, the diagram of cooling curve in every grid-point of a specimen is possible to found out.

$$t_M = \sum_{m=1}^{M} \Delta t_m \tag{3}$$

where M is the number of time steps during the cooling from 800 to 500°C.

Before setting of model of temperature field change in an isotropic rigid body input data, i.e., specific heat capacity of steel, c, heat conductivity coefficient of steel, λ, steel density, ρ, heat transfer coefficient of quenchant, α must be consistent with the achieved results of microstructure and mechanical properties. Optimization of input data should be done according to achieved results. If the variables ρ and c were accepted, variable λ and specially variable α must be estimated, i.e., calibrated according to variables ρ and c. Input values of heat transfer and heat conductivity coefficients can be optimized using Crafts-Lamont diagrams for large spectra of a specimen bar diameter. Heat transfer coefficients of quenchants with different Grossmann severity of quenching were estimated simultaneously with estimation of heat conductivity coefficients of characteristic microstructure constituent [16].

3. Computer modelling of microstructure composition

Contents of ferrite, pearlite, bainite, martensite and austenite at some temperature can be estimated using the diagram in the Figure 1.

Characteristic cooling times in Figure 1 are equal to:

$$t_1 = t_{M95} \tag{4a}$$

$$t_2 = \exp(\log t_{M95} + 0.25(\log t_{M50} - \log t_{M95})) \tag{4b}$$

$$t_3 = \exp(\log t_{M95} + 0.75(\log t_{M50} - \log t_{M95})) \tag{4c}$$

$$t_4 = \exp(\log t_{M50} + 0.25(\log t_{P100} - \log t_{M50})) \tag{4d}$$

$$t_5 = \exp(\log t_{M50} + 0.75(\log t_{P100} - \log t_{M50})) \tag{4e}$$

$$t_6 = \exp(\log t_{P100} + 0.25(\log t_{P50} - \log t_{P100})) \tag{4f}$$

$$t_7 = \exp(\log t_{P100} + 0.75(\log t_{P50} - \log t_{P100})) \tag{4g}$$

where t_{M95}, t_{M50}, t_{P100}, t_{P50} are cooling time from 800 to 500°C for characteristic points in Jominy specimen with 95% of martensite, 50% of martensite, 100% of pearlite and 50% of pearlite in microstructure, respectively. Hardness of characteristic steel microstructure was calculated by equations (5) (Table 1).

Table 1.
Hardness of characteristic steel microstructure

Microstructure	Hardness	
95 % martensite + 5 % bainite	$HRC_{M95} = 0.93HRC_{max}$	(5a)
50 % martensite + 50 % bainite	$HRC_{M50} = 0.73HRC_{max}$	(5b)
100 % pearlite	$HV_{P100} = 0.2308HV_{max} + 100$	(5c)
50 % pearlite + 50 % ferrite	$HV_{P50} = 0.1504HV_{max} + 100$	(5d)

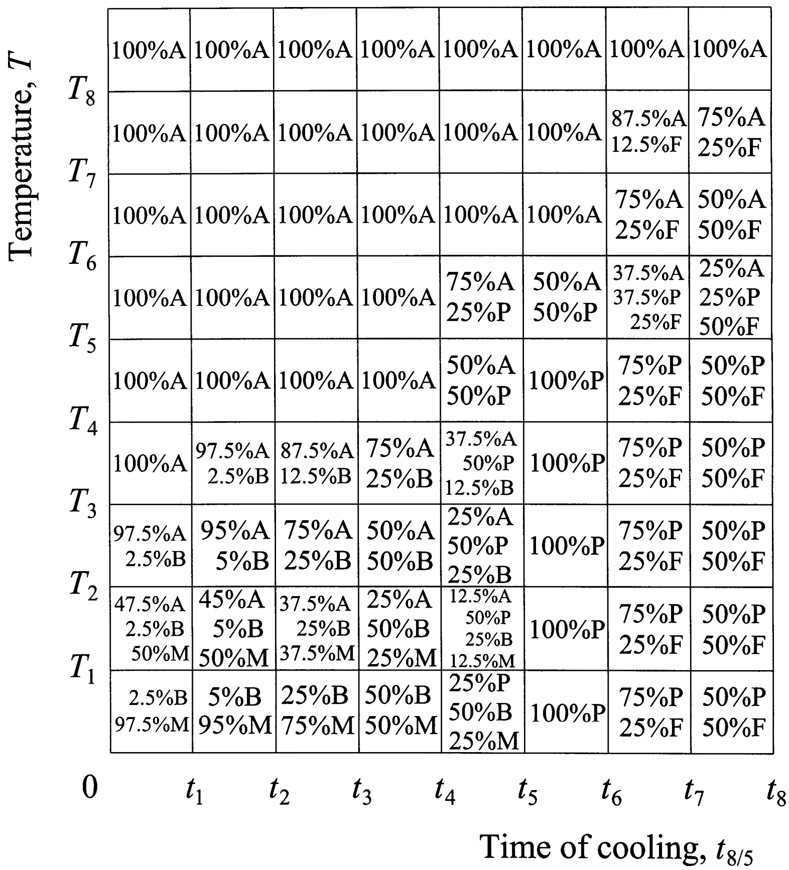

Fig. 1. Contents of ferrite, pearlite, bainite, martensite and austenite at some temperature

Characteristic temperatures in diagram shown in Figure 1 are equal to:

$$T_1 = M_s - 0.75(M_s - M_f) \tag{6a}$$
$$T_2 = M_s - 0.25(M_s - M_f) \tag{6b}$$
$$T_3 = B_s - 0.75(B_s - M_s) \tag{6c}$$
$$T_4 = B_s - 0.25(B_s - M_s) \tag{6d}$$
$$T_5 = A_1 - 0.75(A_1 - B_s) \tag{6e}$$
$$T_6 = A_1 - 0.25(A_1 - B_s) \tag{6f}$$
$$T_7 = A_3 - 0.75(A_3 - A_1) \tag{6g}$$
$$T_8 = A_3 - 0.25(A_3 - A_1) \tag{6h}$$

where M_s is temperature of start of martensitic transformation, M_f is temperature of finish of martensitic transformation, B_s is temperature of start of bainitic transformation, A_1 is equilibrium temperature of eutectoid transformation, A_3 is equilibrium temperature at which transformation of austenite to ferrite begins.

Between critical temperatures A_3, B_s, M_s and M_f of austenite decomposition and hardenability properties, regression relations are established [16]:

$$A_3 = 862 - 0.04(\mathrm{HRC}_{\mathrm{max.}} - 20)^2 - \frac{2.5t_{8/5}}{\mathrm{HRC}_{\mathrm{max}} - 20} \tag{7a}$$
$$B_s = 586 - 0.02(\mathrm{HRC}_{\mathrm{max}} - 20)^2 - \frac{12t_{8/5}}{\mathrm{HRC}_{\mathrm{max}} - 20} \tag{7b}$$
$$M_s = 502 - 0.09(\mathrm{HRC}_{\mathrm{max}} - 20)^2 - \frac{3.5t_{8/5}}{\mathrm{HRC}_{\mathrm{max}} - 20} \tag{7c}$$
$$M_f = 502 - 0.2(\mathrm{HRC}_{\mathrm{max}} - 20)^2 - \frac{3.5t_{8/5}}{\mathrm{HRC}_{\mathrm{max}} - 20} \tag{7d}$$

It was accepted that equilibrium temperature of eutectoid transformation A_1 is equal to 721 °C.

4. Application example

The established relations were applied in computer simulation of microstructure distribution of forged steel centrifugal casting pipe mould made of steel EN 42CrMo4. Computer simulation of hardness and microstructure distribution of the as quenched workpiece was done using the computer software BS-QUENCHING [13].

The shaft was quenched from 850 °C for 45 min/oil with *H*-value equal to 0.2 and tempered at 480°C for 60 min/air. The chemical composition of investigated shaft is: 0.38%C, 0.23%Si, 0.64%Mn, 0.019%P, 0.013%S, 0.99%Cr, 0.16%Mo. Jominy test results of the investigated steel are shown in Table 2.

The geometry of centrifugal casting pipe mould pipe is shown in Figure 2. The microstructure composition in as quenched centrifugal casting pipe mould pipe is shown in Figures 3-5.

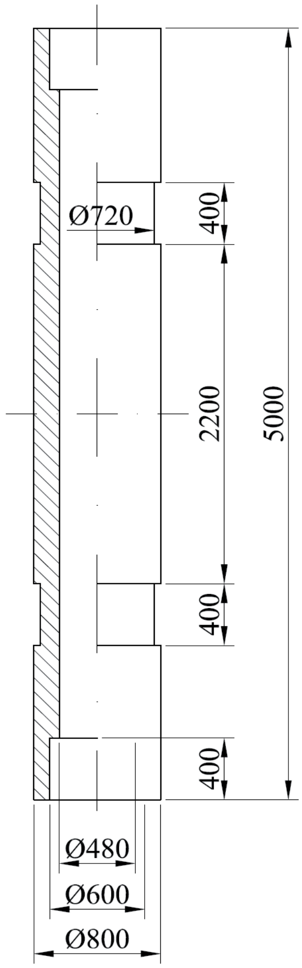

Fig. 2. Geometry of the pipe mould

Table 2.
Jominy test results of steel EN 42CrMo4

Jominy distance/mm	1.5	3	5	7	11	15	20	25	30	40	50
Hardness HRC	55	54	54	53	49	45	39	35	33	31	29

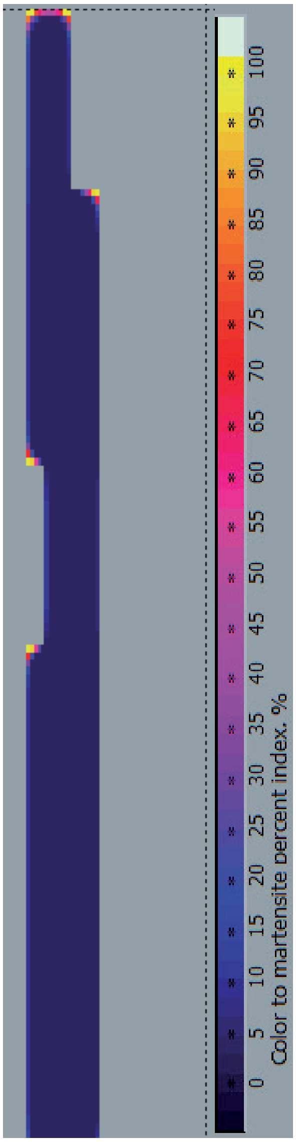

Fig. 3. Distribution of martensite in quenched pipe mould

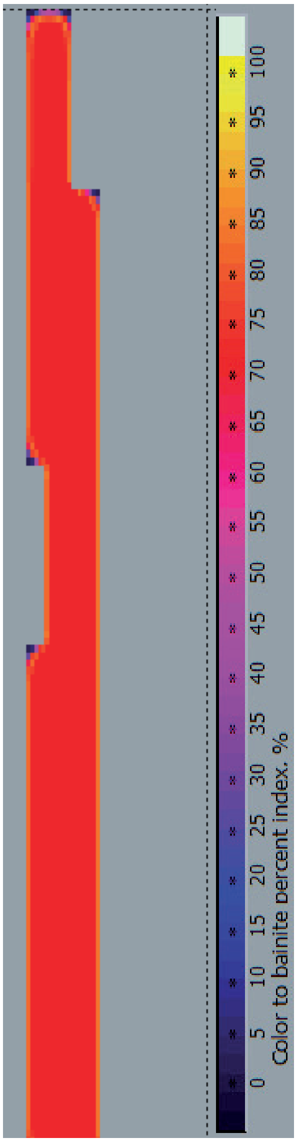

Fig. 4. Distribution of bainite in quenched pipe mould

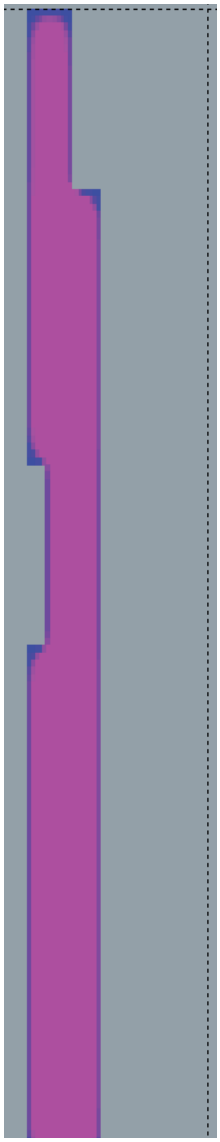

Fig. 5. Distribution of pearlite in quenched pipe mould

5. Conclusions

Input material data involved in mathematical model of transient temperature field, i.e., density and specific heat capacity of steel was accepted from literature. Heat transfer coefficient and heat conductivity coefficient have been successfully calibrated by using results of quenching given in Crafts-Lamont diagrams. Using a Crafts-Lamont diagrams, heat transfer and heat conductivity coefficients are predicted by inversion method, i.e. by mathematical modelling of quenching of steel bars.

A developed mathematical model has been applied in computer simulation of quenching of steel shaft, as well as, of die component of high hardenability steel. It can be concluded, that hardness and microstructure composition in quenched steel can by successfully calculated by proposed method.

Acknowledgements

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