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Computer simulation of mechanical properties, stresses and strains of quenched steel specimen

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Analysis and modelling

ABSTRACT

Purpose: The research purpose is to upgrade the mathematical modelling and computer simulation of thermal processing of materials.
Design/methodology/approach: Based on theoretical analyze of physical processes which exist in quenching systems the proper mathematical model is established and computer software is developed.
Findings: On the basis of control volume method the algorithm for prediction of hardness distribution, residual stresses and strains in quenched steel specimens with complex geometries have been established. The mathematical model of steel hardening is consisted of numerical calculation of temperature field change in process of cooling, and of numerical simulation of hardness. The hardness has been predicted by the conversion of calculated time of cooling from 800ºC to 500ºC to hardness results, using the Jominy hardenability curve.
Research implications: The algorithm is completed to solve 2-D situation problems such as the quenching of complex cylinders, cones, spheres, etc. Surface heat transfer coefficient was obtained by the calibration.
Practical implications: The established model of steel quenching could be successfully in the practice of heat treatment.
Originality/value: The established method in efficient approach combines the no expensive experimental Jominy-test and computer simulation in prediction of mechanical properties and behaviour of steel during the quenching.
Keywords: Numerical techniques; Computer simulation; Quenching

1. Introduction

Steel quenching could be defined as “cooling of steel workpieces at a rate faster than still air” [1]. Although, very simple on first sight, quenching is physically one of the most complex processes in engineering, and very difficult for understanding. Quenching used to be called the black hole of heat treatment processes [2, 3].

All of the heat treatment processes are more and more sophisticated and require to be accurately defined. Computer simulation of heat treatment processes provides evaluation physical quantities important for accurate definition of heat treatment processes.

Generally, in simulation of steel quenching, two essential problems have to be solved. The first problem is to develop mathematical model of cooling and mechanical properties prediction and second problem is how to establish the proper method for real heat data evaluation [4, 5].

Computer simulation of quenching includes several different analyses: (1) heat transfer analysis - computation of cooling curves, (2) material properties analysis - computation of microstructure composition and mechanical properties, (3) thermoplastic analysis - computation of stresses and strains and (4) fracture mechanics analysis - computation of damage tolerance [1, 6].

Simulation of anyone process could be made successfully only if all mechanisms of process are well known and if the appropriate mathematical methods are used. It means for steel quenching that the essential characteristics of the phase transformation and mechanisms of stress and strain generation during the quenching should be known. In steel quenching stress-strain analyse, both, strains due to thermal strain and strains due to phase changes have to be taken in account [1]. Values of physical and mechanical, properties as functions of microstructure and temperature should be known at everyone moment during the quenching [7]. From these reasons it is understandable that computer simulation of steel quenching is of interest to engineers from a wide range of disciplines, i.e., material science, thermodynamics, mechanics, manufacturing, mathematics, chemistry, etc.

Detailed theoretical and quantitative analysis of the process that can be applied to a wide range of different component types quenching remains unavailable. Although many attempts have been made to develop theoretical models to describe the steel quenching, all the earlier work relied on simplifications that rendered the analysis unrealistic. In particular, successful describe the steel quenching is not possible before good theoretical explanation all of physical processes involved in mathematical model. Second, the real complexities of plasticity have to be introduced into the model, but it has known that the theory of plasticity is not sufficient developed. Moreover, the variation of physical and mechanical properties with temperature could be involved in mathematical model.

In the past three decades the Finite Element Method (FEM) has enjoyed an undivided popularity as the method for solid body stress analysis. On the other hands the Finite Volume Method (FVM) has been established as a very efficient way of solving heat transfer problems. Recently FVM is used as a simple and effective tool for the solution of a large range of problems in the thermoplastic analysis.

2. Calculation of temperature field

Temperature field change in an isotropic rigid body with heat conductivity λ, density ρ, and specific heat capacity c can be described by Fourier's low of heat conduction:

$$\frac{\partial(c\rho T)}{\partial t} = \mathrm{div}\,\lambda\,\mathrm{grad}\,T \tag{1}$$

In equation (1) heat sources that can exist during the steel quenching is neglected.

For steel quenching initial condition is:

$$T(r,z,t=0) = T_a \tag{2}$$

and characteristic boundary condition is:

$$-\lambda\frac{\partial T}{\partial n}\Big|_s = \alpha(T_s - T_f) \tag{3}$$

where: T_a - austenitising temperature of, K
T_f - quenchant temperature, K
T_s - boundary temperature, K

Axially symmetrical bodies, as complex cylinders, cones, spheres can be described as 2-D problem in cylindrical coordinates r, z and φ=1.

The discretization equation can be established by using the finite volume formulation, i.e., by integrating the differential equation over each control volume taking in account a initial and boundary condition [8]. Discretization equation is equal [9]:

$$T^1_{ij}\Big(\sum_{m=1}^{2} b_{(i,i+n)j} + \sum_{m=1}^{2} b_{i(j,j+n)} + b_{ij}\Big) = \sum_{m=1}^{2}\Big(b_{(i,i+n)j}T^1_{(i,i+n)j} + b_{i(j,j+n)}T^1_{i(j,j+n)}\Big) + b_{ij}T^0_{ij}$$

$$i=1,2..i_{\max} \quad j=1,2..j_{\max} \qquad n=3-2m \tag{4}$$

where:
$b_{ij} = Q_{ij}\Delta t^{-1}$, variable Q_{ij} is heat extracted during the time step Δt; $b_{(i,i+n)j} = W_{(i,i+n)j}^{-1}$ and $b_{i(j,j+n)} = W_{i(j,j+n)}^{-1}$, variable $W_{(i,i+n)j}$ is the thermal resistance between ij and $i+n,j$ volume and variable $W_{i(j,j+n)}$ is the thermal resistance between ij and $i,j+n$ volume ($n = 1$).

Discretization system in equation (3) has N linear algebraic equations with N unknown temperatures of control volumes, where N is number of control volumes. Time of cooling from T_a to specific temperature in particular points is determined as sum of time steps and cooling curve in every grid-point of a specimen can be calculated.

Physical properties c and ρ were directly accepted from relevant references and physical properties λ and α are estimated by using the calibration method described in reference [10] and [11]. Temperature dependencies of heat transfer coefficients have been calibrated on the basis of Crafts-Lamont diagrams.

3. Mathematical modelling of the phase transformations and mechanical properties

The structural transformations and mechanical properties were estimated based on time, relevant for structure transformation. The characteristic cooling time, relevant for structure transformation in most structural steels is the time of cooling from 800 to 500 ºC (time $t_{8/5}$) [9, 12, 13]. The hardness at grid-points is estimated by the conversion of cooling time $t_{800/500}$ results to hardness by using the relation between *cooling time* and *distance from the quenched end of Jominy specimen* shown in Figure 1 [14].

Involving the time $t_{8/5}$ in the mathematical model of steel hardening, the *Jominy*-test result could be involved in model. *Jominy*-values can be experimentally evaluated or calculated from elemental composition. Since all the alloying elements have a cumulative effect on hardenability, it is essential that all elements, including residuals, be taken into account. Hardenability depends also on the degree of solution of the carbides and it cannot be accurately predicted only from elemental composition. The grain size at the temperature of austenitization must be known in calculation of *Jominy*-values.

Structure composition and mechanical properties were predicted on the basis of calculated hardness in grid-points. Characteristic temperatures of microstructure transformation were predicted by the inversion method from the predicted structure composition.

Mechanical properties of quenched steel, and also, mechanical properties of quenched and tempered steel, directly depends on degree of quenched steel hardening [15]. Mechanical properties were estimated from HV hardness by using methods explained in reference [9].

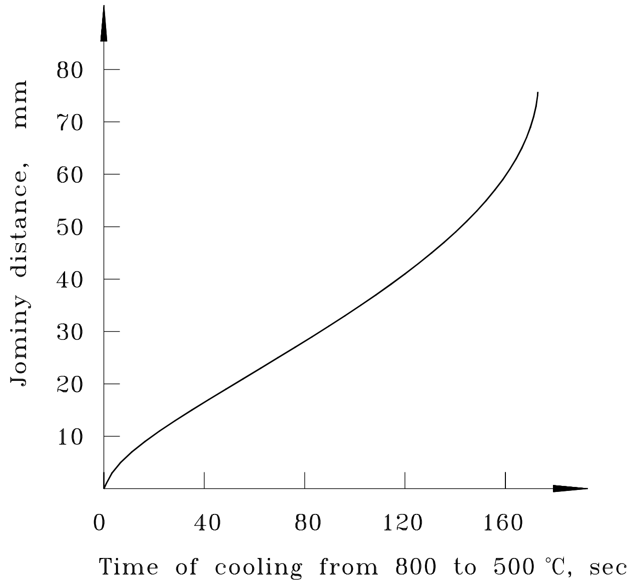

Fig. 1. Cooling time from 800 to 500 °C vs. distance from the quenched end of *Jominy*- specimen

4. Calculation of stresses and strains during the quenching

The equilibrium and compatibility equations in thermoelastic-plastic analyse are independent of the plasticity relations.

The equilibrium relations in tensor notation are:

$$\sigma_{ij,i} = -F_i \qquad \sigma_{ij} = \sigma_{ji} \tag{5}$$

Body forces are equal zero during the quenching. Components undergoing the heat treatment are not restrained at the surfaces.

Prnadtl-Reuss plastic flow rule and Von-Mises principle hardening condition were accepted to established constitutive equation of elastic-plastic model. In the elastic-plastic analyse the strain of transformation plasticity has been taken in account.

If the assumed that the total strain is the sum of the elastic and plastic strains then relationships between stress and strain are expressed by a total of six equations:

$$\varepsilon_{ij} = \frac{1}{2G}\sigma_{ij} - \delta_{ij}\left(\frac{\mu}{E}\Theta - \alpha T - \varepsilon_{st}\right) + \varepsilon_{ij}^{pl} \tag{6}$$

where $G = E/2(1+\mu)$; $\Theta = \sigma_{ii}$; E-modulus of elasticity; μ-Poisson`s ratio, α-linear coefficient of thermal expansion. Plastic strain increments could be equal:

$$d\,\varepsilon_{ij}^{pl} = \frac{3}{2}\frac{S_{ij}}{\sigma_e}d\,\varepsilon_{pl}$$
$$\sigma_e = \sqrt{\frac{3}{2}S_{ij}S_{ij}}, \qquad d\,\varepsilon_{pl} = \sqrt{\frac{3}{2}d\,\varepsilon_{ij}^{pl}\,d\,\varepsilon_{ij}^{pl}} \tag{7}$$

where S_{ij} - deviator stress tensor, σ_e-equivalent modified stress, ε_{pl} -equivalent modified total strain. σ_e and ε_{pl} could be estimated from true-stress - true-strain curve. The six strain components are related to the displacements by:

$$\varepsilon_{jk} = \frac{1}{2}(u_{k,j} + u_{j,k} - u_{i,j}u_{i,k}) \tag{8}$$

In order to carry out such calculations it is necessary to posses a set of relationships between temperature and position at various times during the cooling process as well as the relationships between temperature and material properties. Thus in general there are 15 unknowns, but there are in turn 15 equations which relate these unknowns in the *x,y,z* coordinate system.

The discretization equation can be established by using the finite control volume formulation, i.e., by integrating the differential equation over the each control volume [9].

Discretization equation for each control volume can be established by expressing the stresses from displacements and integrating the differential equation over the each control volume. System of 2N linear algebraic equations with 2N unknown displacements can be formed, where N is number of control volumes. For example, the discretizated equilibrium equation in *x* direction for a 2-D situation is equal:

$$a_p u_p = \sum_k a_k u_k + b$$
$$a_p = \sum_k a_k \qquad k = l,r,t,b \tag{9}$$

The coefficients a_k and b are equal:

$$a_r = [(\lambda + 2G)\frac{S}{\delta x}]_r, \quad a_l = [(\lambda + 2G)\frac{S}{\delta x}],$$
$$a_t = (G\frac{S}{\delta y})_t, \quad a_b = (G\frac{S}{\delta y})_b, \tag{10}$$

$$b = [\frac{\lambda S}{\delta y}(v_t - v_b)]_r - [\frac{\lambda S}{\delta y}(v_t - v_b)]_l + [\frac{GS}{\delta x}(v_r - v_l)]_t -$$
$$-[\frac{GS}{\delta x}(v_r - v_l)]_b - \frac{\alpha E}{(1 - 2\mu)}[(ST)_t - (ST)_b] \tag{11}$$

where: $S_{(r,l,t,b)}$ is characteristic volume surface; $\delta x_{(r,l,t,b)}$ and $\delta y_{(r,l,t,b)}$ are characteristic finite volume dimensions; λ and G are Lame´s coefficients.

5. Numerical verification

Numerical calculations and experimental investigations of steel specimen hardening were made in order to test performance of established mathematical model. Hardening was achieved on the specimen with a complex geometry. Experimentally evaluated *Jominy*-results of investigated steel are shown in Table 1.

Heat treatment for quenching of the steel 60WCrV7 was: heating on 880 ºC for 25 min and oil quenching.

The specimen was quenched in agitated oil with the severity of quenching, i.e., *Grossmann's* H-value equal to 0.25.

Calibrated characteristic values of heat transfer coefficient of oil with H-value equal to 0.25 vs. surface temperature are shown in Figure 2.

Table 1.
Jominy-test results

J-distance, mm	0	5	7.5	10	12.5	15	17.5	20	25	30	40	50
Hardness, HRC	62	62	60	54	50	45	42	41	40	38	37	35

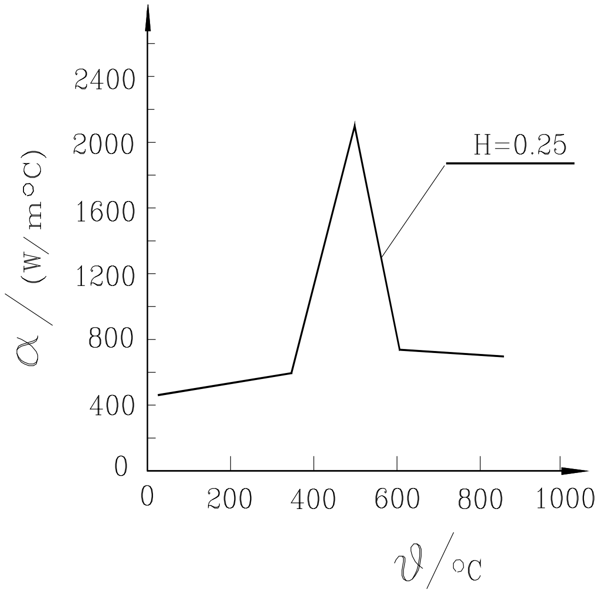

Fig. 2. Calibrated values of heat transfer coefficient

Figure 3 shows computed and experimentally estimated result of HRC hardness of the hardened specimen. The values of experimentally estimated hardness are converted from HV hardness to HRC hardness. Differences between experimentally and numerically estimated hardness penetration depths have been negligible. Computer simulation of distortions generated during the quenching is shown in Figure 4. Distortions are shown in magnification 100:1.

Experimentally defined total distortion at the location of the largest diameter was equal 0.1mm, i.e., 2 · 0.05 mm and longitudinal distortion was 0.13 mm.

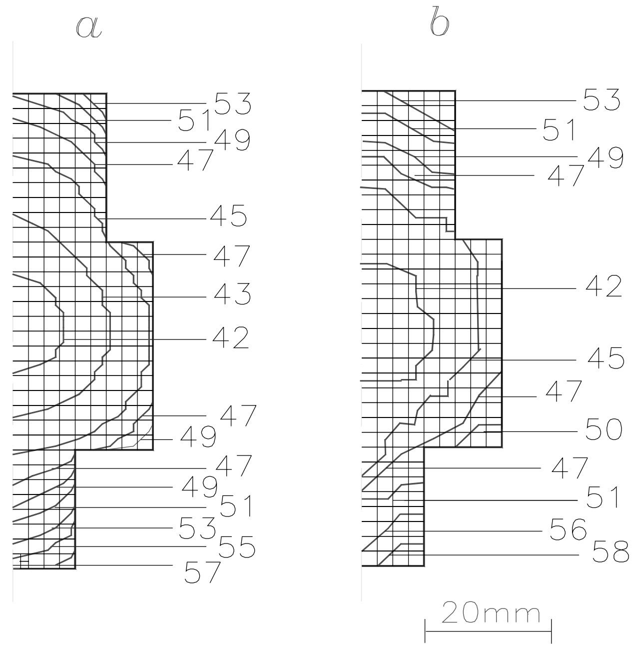

Fig. 3. Hardness distribution: (a) computer simulation, (b) experiment

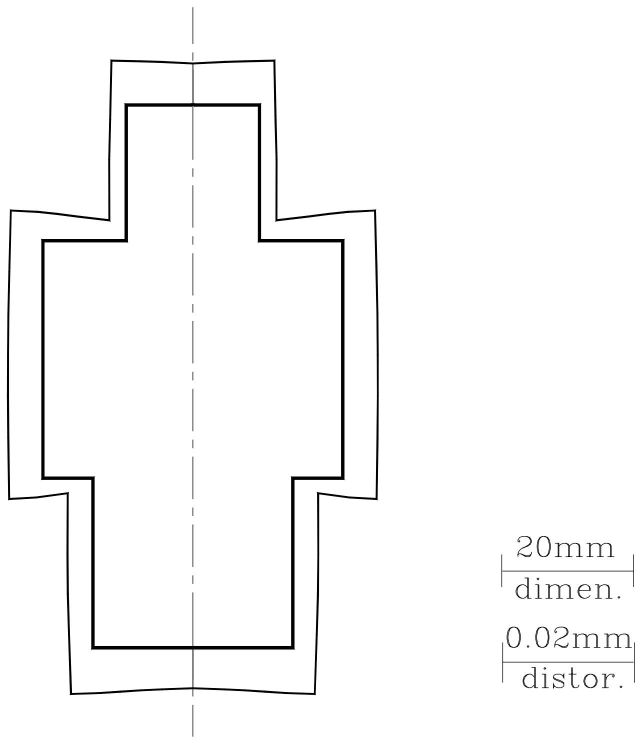

Fig. 4. Computer simulation of distortion

6. Conclusions

A mathematical model of steel hardening has been developed to describe the hardness distribution in a steel specimen with complex geometry. The model is based on the control volume method. It consists of numerical calculation of temperature fields in process of cooling, and of numerical simulation of mechanical properties.

The time of cooling of steel specimens can be successfully estimated by using the calibrated values of heat transfer coefficients that have been used in the mathematical model.

The relevant cooling process of a specimen can be well presented by time of cooling from 800 to 500ºC and hardness distribution can be effectually estimated on the basis of time of cooling from 800 to 500ºC, i.e., by the conversion of mentioned specific time to hardness results using the *Jominy*-test results.

The established model has been successfully applied in computer simulation of mechanical properties and distortions of the quenched specimen with complex form. Differences between calculated and experimentally defined hardness and distortions of investigated case were negligible.

The finite volume method is a good numerical method for computer simulation of temperature field, mechanical properties, residual stresses and strains of the quenched steel workpiece.

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