Computer simulation of mechanical properties and distortions during the quenching of steel

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Abstract. The research main stream in this paper is to upgrade the mathematical modelling and computer simulation of quenching of steel. Based on theoretical analyse of physical processes which exist in quenching systems of steel workpieces, the mathematical model for computer simulation mechanical properties and distortions during the quenching has been developed. The mathematical model of steel quenching is focused on physical phenomena such as heat transfer, phase transformations, mechanical properties and generation of stresses and distortions. Because of that the numerical procedure of computer simulation of steel quenching is divided in three parts: numerical calculation of transient temperature field, numerical calculation of phase change and numerical calculation mechanical behaviours of steel. The numerical procedure is based on control volume method. Relevant physical properties about which cooling rate depends are specific heat capacity of steel, heat conductivity coefficient of steel, steel density, linear thermal expansion, transformation expansion, and heat transfer coefficient of quenchant. Also, the transformation plasticity has been included in the model. Physical and mechanical properties that were included in such model have been predicted by taking into account their temperature dependences. In the developed computer program for simulation quenching the hardness at different workpiece points is estimated by the conversion of the calculated cooling time from 800 to 500 °C, \( t_{8/5} \) to the hardness by using both, the relation between cooling time, \( t_{8/5} \) and Jominy distance and the Jominy hardenability curve. Other properties of steel have been estimated based on as quenched hardness of steel. Based on the developed algorithm, computer software is developed for simulation of 3D situation problems, such as the quenching of complex cylinders, cones, spheres, etc., can be simulated. The established numerical model and computer software for simulation of steel quenching can be successfully applied in the practical usage of quenching.

1. Introduction
Research of numerical modelling of residual stresses, distortion distribution is one of the priority researches in simulation of phenomena of steel quenching [1]. There is necessary to establish the appropriate algorithm which describes heat transfer, physical and mechanical properties, microstructures, residual stresses and distortions.

Rate of steel specimen cooling essentially depends on both, workpiece geometry and characteristic physical properties of quenched steel and quenchant and thermal boundary conditions. Inverse
physical problems should be solved to determine mechanical and thermal properties of materials based on experimentally evaluated results [1-3].

Distribution of mechanical properties steel can be successfully predicted based on Jominy test results by inversion methods [4]. In this method the evolution of temperature should be simulated using the numerical methods. Then the characteristic time of cooling from 800 to 500 C degree, time \((t_{8/5})\) for chosen point can be extracted from the simulation results. The equivalent cooling time \(t_{8/5}e\) can be used instead of cooling time \(t_{8/5}\). Equivalent cooling time \(t_{8/5}e\) is function of cooling time, \(t_{8/5}\) and history of cooling. The characteristic times then should be converted to equivalent distances on the Jominy test specimen. Finally, the distribution of the microstructure and mechanical properties, hardness, yield strength, tensile strength, elongation, and impact toughness can be predicted by transferring the hardness of Jominy specimen results to the points of steel specimen sharing the same characteristic time [6]. Simulations of microstructural transformations during the quenching should be supported by the CCT diagrams using linear alignment with the actual chemical composition [7]. Regression relations between critical temperatures of austenite decomposition and hardenability properties were established, in Ref. [7, 8].

The numerical elastoplastic problem for evaluation residual stresses and distortions cold be solved by application of the Ilyushin method of successive elastic solutions. In the elastic-plastic analysis thermal strain, strains due to transformations and strain of transformation plasticity has been taken into account [8].

Finite volume method (FVM) is a simple and effective tool for the solution of a large range of problems in the analysis of thermal processes [9, 10]. The discretization system was established by using the finite volume formulation.

2. Computer modelling of heat transfer
The temperature field change in an isotropic rigid body with coefficient of heat conductivity, \(\lambda\), Wm\(^{-1}\)K\(^{-1}\), density, \(\rho\), kgm\(^{-3}\) and specific heat capacity, \(c\), Jkg\(^{-1}\)K\(^{-1}\) can be described by Fourier’s law of heat conduction:

\[
\frac{\partial(c\rho T)}{\partial t} = \text{div}\lambda \text{ grad}T + q'
\]

Characteristic boundary condition is:

\[
-\lambda \left| \frac{\partial T}{\partial n} \right| = \alpha(T_s - T_f)
\]

where \(T\), \(K\) is the temperature, \(t\), \(s\) is the time, \(T_s\), \(K\) is surface temperature, \(T_f\), \(K\) is quenchant temperature, \(\alpha\), Wm\(^{-1}\)K\(^{-1}\) is heat transfer coefficient.

The internal heat source due to latent heat, \(q'\), Jm\(^{-3}\)s\(^{-1}\) which is a function of transformation rate and temperature is equal to \(q' = \Delta H_{a\beta}x'_{a\beta}\), where \(\Delta H_{a\beta}\) is the latent heat of transformation phase \(a\) to phase \(\beta\) and \(x'_{a\beta}\), m\(^{3}\)s\(^{-1}\) is the phase transformation rate. Input data, i.e., specific heat capacity, \(c\), heat conductivity coefficient, \(\lambda\), density, \(\rho\) of all microstructural constituents, and heat transfer coefficient of quenchant, \(\alpha\) must be consistent with the experimentally achieved results of microstructure and mechanical properties of quenched steel. Values of density, \(\rho\) and specific heat capacity, \(c\) can be accepted from literature [7]. The estimation of input values of heat transfer coefficient can be optimized using Crafts-Lamont diagrams [11]. Relations which exist between heat conductivity coefficient, \(\lambda\) and some indicators of hardenability were studied on numerous steels with different chemical composition. Regression relations for heat conductivity coefficients at different temperature as well as for different microstructure constituents are expressed. Total heat conductivity coefficients of steel at some temperature, \(T\) were estimated by [7]:

\[
\lambda_T = f(x_F, x_P, x_B, x_M, x_A, \lambda_{(P+P)}^\beta, \lambda_B^\beta, \lambda_M^\beta, \lambda_A^\beta)
\]
Solution of Eq 1 can be found out using the finite volume method [12]. If the total volume is divided in N number of control volumes, discretization system has N linear algebraic equations, with N unknown temperatures 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 find out.

\[
T_M = \sum_{m=1}^{M} \Delta t_m
\]  

(4)

3. Prediction of Hardness and Microstructure Composition

Simulation of as quenched hardness at different workpiece points is estimated by the conversion of the calculated cooling time, \( t_{8/5e} \) to the hardness. This conversion is provided using the relationship between the cooling time \( t_{8/5e} \) and distance from the quenched end of the Jominy test specimen, \( E \), i.e. by the using the diagram of cooling time \( t_{8/5} \) versus distance from the quenched end of the Jominy test specimen [11].

\[
E = f(t_{8/5e})
\]  

(5)

As-quenched hardness HRC\(_q\) was predicted by using the Jominy curve diagram:

\[
\text{HRC}_q = f(E_d)
\]  

(6)

Microstructure composition after the quenching depends on chemical composition of steel and nature of cooling process. In the same time Jominy values can be experimentally evaluated or calculated from elemental composition. Regression relations between microstructure composition, steel hardness and hardness of microconstituents in one side and characteristic Jominy-hardness, Jominy-distances, and shape of Jominy curve in other side were find out. In this way the microstructure composition and mechanical properties if steel can be predicted based on Jominy test results by inversion method. For this purpose, the cooling curves of the Jominy specimen should be predicted by numerical methods [4]. In this approach microstructure composition can be found out by inversion method using the Jominy test results.

Microstructure composition after the quenching depends on chemical composition of steel and nature of cooling process. Kinetics of transformations was calculated by Avrami’s isothermal equation. Transformed part of microstructure, \( X \) is equal to:

\[
x = 1 - \exp(-k \cdot t^n) \]

(7)

Kinetic parameters \( k \) and \( n \) from Eq 7 can be determined inversely by using data about the time of isothermal transformation, \( t_T \).

\[
k = \frac{\ln(1 - x)}{t_T^n}
\]  

(8)

For purpose of numerical analysis by computer, it is convenient when kinetics of austenite decomposition is defined in an incremental form. The Avrami’s isothermal equation can be written in an incremental form and the volume fraction, \( \Delta X \) of austenite transformed in the time interval \( \Delta t_i \) at temperature \( T_i \) can be calculated as follows:

\[
\Delta X_{(m)} = nk^n \left( \ln \frac{1}{1 - X_{(m-1)}} \right)^{-\frac{1}{n}} (1 - X_{(m-1)}) \Delta t_{(m)}
\]  

(9)
In accordance to the Scheil’s additivity rule, characteristic microstructure transformation is finished when transformed part of microstructure, $\Sigma \Delta X$ is equal to one [13, 14].

$$\sum_{m=1}^{M} nk^n \left( \ln \frac{1}{1 - X_{(m-1)}} \right)^{1-n} \left( 1 - X_{(m-1)} \right) \Delta t_{(m)} = 1$$  \hspace{1cm} (10)

The non-isothermal transformation kinetics can be described as the sum of a series of the small isothermal transformations. The IT diagram should be additionally adjusted based on actual chemical composition or based on Jominy test results for applied steel [4].

Increment of martensite $\Delta x_M$ in temperature depth $\Delta T = T_m - T_{m-1}$ is equal to:

$$\Delta x_M = x_M(T_{m+1}) - x_M(T_m)$$  \hspace{1cm} (11)

Quantity of martensite $x_M$ at temperature $T$ is equal to [15]:

$$x_M = (1 - x_F - x_P - x_B)[1 - \exp(-0.011(M_s - T))]$$  \hspace{1cm} (12)

where F, P and B represent ferrite, pearlite, and bainite, respectively.

Between critical temperatures of austenite decomposition and hardenability properties, regression relations are established in Ref. [7].

4. Prediction of Mechanical Properties

Mechanical properties of steel during quenching directly depend on the degree of quenched steel hardening and temperature [16, 17]. Mechanical properties, yield strength, $R_e$, tensile strength, $R_m$, Poisson’s coefficient, $\nu$, modulus of elasticity, $E$, strain-hardening coefficient, $K$ and strain-hardening exponent, $n$ could be estimated from hardness HRC or HV [6].

$$\text{Mechanical property} = f(\text{HV Hardness, Microstructure composition, Temperature})$$  \hspace{1cm} (13)

Mechanical properties of quenched steel or quenched and tempered steel directly depends on degree of quenched steel hardening [6]. One most tested relation in material science is relation between hardness and ultimate tensile stress. Relation between hardness HV and ultimate tensile stress, $R_m$, MPa is equal to:

$$R_m = 3.3HV$$  \hspace{1cm} (14)

By experimental work it was found out that relation given by equation (14) is valid for tensile strength range between 400-2500 MPa [18].

Relation between hardness HV and yield strength, $R_e$, MPa is equal to [17]:

$$R_e = (0.8 + 0.1S)R_m + 170S - 200$$  \hspace{1cm} (15)

Coefficient $S$ which is ratio between the actual hardness and hardness of martensite in Rockwell C hardness, should be taken in account since as-quenched and quenched and tempered steel properties depends on degree of quenched steel hardening [6, 19].

The strain-hardening exponent, $n$ can be defined by [20]:
\[
\frac{R_m}{R_e} \left( \frac{n}{0.002e} \right)^n \approx 0
\]

(16)

The definition of dependence of flow stress, \(\sigma_{\text{flow}}\), on temperature can be expressed by [21]:

\[
\sigma_{\text{flow}} = C_2 e^{Q/RT}
\]

(17)

where \(Q\) is an activation energy for plastic flow; \(R\) is the universal gas constant; \(C_2\) is empirical constant; and \(T\) is the absolute temperature. For carbon steel of 0.2 % C, constant \(C_2 = 146\) N/mm\(^2\) and \(Q = 2,290\) J/Kmol.

5. Prediction of Residual Stresses and Distortions

Formulation of mechanical field should satisfy the equilibrium relations. The equilibrium relations in tensor notation are:

\[
\sigma_{ij,i} = -F_i
\]

\[
\sigma_{ij} = \sigma_{ji}
\]

(18)

Components undergoing the heat treatment are not restrained at the surfaces. In the elastic-plastic analysis the strains due to transformations and strain of transformation plasticity has been taken into account. If it is assumed that the total strain is the sum of the elastic strain, plastic strain, thermal strain, strain due to phase transformation, and transformation plasticity strain, then relationships between stress and strain are expressed by a total of six equations. Prandtl-Reuss plastic flow rule and Von-Mises principle hardening condition were accepted to established constitutive equation of the elastic-plastic model [20]:

\[
\varepsilon_{ij,i} = \frac{1}{2G} \sigma_{ij} - \delta_{ij} \frac{\mu}{E} \Theta - \varepsilon_{ij}^m + \varepsilon_{ij}^p + \varepsilon_{ij}^{\theta p}
\]

(19)

where \(G = E/(1 + \mu)\); \(E\) is modulus of elasticity; \(\mu\) is Poisson’s ratio; \(\Theta = \sigma_{ij}\). Plastic deformation in incremental formulation is equal to:

\[
\varepsilon_{ij}^p = \sum_{m=1}^{k-1} \Delta \varepsilon_{ij,m}^p + \Delta \varepsilon_{ij,k}^p
\]

(20)

The plastic strain increments \(\Delta \varepsilon_{ij,k}^p\) are related to the stresses through the yield criterion [20]:

\[
\Delta \varepsilon_{ij}^p = \frac{3}{2} \frac{\Delta \varepsilon_{ij}^p}{\sigma_e} \sigma'_{ij}
\]

(21)

where

\[
\Delta \varepsilon_{ij} = \frac{2}{3} \Delta \varepsilon_{ij}^p \Delta \varepsilon_{ij}^p
\]

\[
\sigma_e = \frac{3}{2} \sigma'_{ij} \sigma'_{ij}
\]

(22)

(23)

where \(\sigma'_{ij}\) is the deviatoric stress, \(\sigma_e\) is equivalent modified stress; and \(\Delta \varepsilon_{ij}^p\) is equivalent modified total strain. Stress \(\sigma_e\) could be estimated from \(\Delta \varepsilon_{ij}^p\) by using the true stress-strain curve. True stress-strain curve can be predicted by Eqs 16 and 17.
Thermal strain increment due to thermal expansion is defined as:

$$
\varepsilon_{ij}^T = \sum_{m=1}^{M} \sum_{k=1}^{p} \delta_{ij} x_k \alpha_{km} \Delta T_m
$$

(24)

where $\alpha_{km}$ is the temperature-dependent thermal expansion coefficient for $k$-phase.

Strain due to a phase transformation can be formulated by:

$$
\varepsilon_{ij}^m = \sum_{m=1}^{M} \sum_{k=1}^{p} \frac{1}{3} \delta_{ij} \beta_k \Delta x_k
$$

(25)

where $\beta_k$ represents the structural dilation due to decomposition of austenite to the $k$th phase.

Transformation plasticity strain can be formulated by Greenwood and Johnson [21] approach combined with a scaling factor for partial transformation as used by Oddy et al. [22]. The used equation is on incremental form written as:

$$
\varepsilon_{ij}^{tp} = \sum_{m=1}^{k} \Delta \varepsilon_{ij,m}^{tp} + \Delta \varepsilon_{ij,k}^{tp}
$$

(26)

$$
\Delta \varepsilon_{ij}^{tp} = \frac{5 \Delta V}{4V} \frac{1}{R_e} \sigma''(2 - 2x_m - \Delta x) \Delta x
$$

(27)

$\Delta \varepsilon_{ij}^{tp}$ is the specific volume change, $R_e$ is the yield stress of the weaker phase, $\sigma''$ is the stress deviator tensor, $\Delta x$ is the transforming fraction and $x_m$ is the fraction already transformed.

The elastoplastic problem can be successfully solved by application of the Ilyushin method of successive elastic solutions. The discretization system can be established by using the finite volume formulation [9]. The six strain components are related to the displacements by:

$$
\varepsilon_{jk} = \frac{1}{2} \left( u_{k,j} + u_{j,k} - u_{j}u_{k,j} \right)
$$

(28)

The discretized equilibrium equation of finite volume can be established by expressing the stresses from displacements, and finally, integrating the differential equation over the control volume. For axial symmetric body a system of $2N$ linear algebraic equations with $2N$ unknown displacements can be formed, where $N$ is number of control volumes.

6. Application Example

Developed model was applied in computer simulation of quenching of cylindrical steel specimen 20 mm diameter by 60 mm long, made of steel JIS S45C shown in Ref. [3]. Standard IT- diagram was adjusted based on Jominy test results. Low values of Jominy curve of standard steel JIS S45C are accepted for research [26]. In purpose of computer simulation it was presumed that specimen was quenched from 850 °C for 30 min/water with Grossmann's H-value equal to 1 Ref. [8].

The distribution of hardness of the as quenched cylindrical steel specimen is shown in figure 1a. The distribution of ferrite, pearlite, bainite and martensite of as quenched should be calculated [11]. The distribution of residual stresses and displacements in the as quenched cylindrical steel specimen is shown in figures 1b-1e. Simulation was done using the computer software BS-QUENCHING [11].
Figure 1. Distribution of a) hardness, b) circumferential stress, c) longitudinal stress, d) radial displacement, e) longitudinal displacement of as quenched steel specimen [8].

The residual stresses and change in diameter are measured at the surface and middle of the length Ref. [3] (table 1).

|                   | Model | Experiment, source: Ref. [3] |
|-------------------|-------|-----------------------------|
| Change of length, mm | 0.096 | 0.110                       |
| Change of diameter, mm | 0.020 | 0.000                       |
| Circumferential stress, MPa | -241  | -124                        |
| Longitudinal stress, MPa | -286  | -311                        |

7. Conclusions
The developed model of quenching is based on the finite volume method and consists mathematical modelling of heat transfer, physical properties, mechanical properties, residual stresses and distortion.

The estimation of input values of heat transfer coefficient were optimized using Crafts-Lamont diagrams. Material properties have been estimated based on hardenability of steel by inversion methods and optimized based on experimentally received Jominy test results.

As quenched hardness at different workpiece points is estimated by the conversion of the equivalent characteristic cooling time from 800 to 500 °C to the hardness using the Jominy test results. The equivalent cooling time \( t_{8/5} \) is function of cooling time, \( t_{8/5} \) and history of cooling during the quenching.

In the elastic-plastic analysis thermal strain, strains due to transformations and strain of transformation plasticity has been taken into account. The numerical elastoplastic problem for evaluation residual stresses and distortions were solved by application of successive elastic solutions. The discretization system was established by using the finite volume formulation.

The quenching of rotationally symmetric steel workpiece was simulated in order to test the possibility of application of developed software. Only a designation of applied steel was known.

By experimental verification of the computer simulation results it have been found out that, phenomena of steel quenching could be successfully described by the proposed computer model. The
developed mathematical model and computer software is suitable for preliminary selection of quenching treatment of steel.

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