Numerical Simulation of Steel Quenching

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The algorithm and computer program are completed to simulate the quenching of complex cylinders, cones, spheres, etc. Numerical simulation of steel quenching is a complex problem, dealing with estimation of microstructure and hardness distribution, and also dealing with evaluation of residual stresses and distortions after quenching. The nonlinear finite volume method has been used in numerical simulation. By the established computer program, mechanical properties and residual stresses and strains distributions in the quenched specimen can be given at every moment of quenching.

Keywords hardenability, hardness, modeling, quenching, simulation, steel properties

1. Introduction

Steel quenching can 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 to understand. Quenching used to be called the black hole of heat treatment processes.[2]

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

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

Simulation of any one process can be made successfully only if all mechanisms of the process are well known and if the appropriate mathematical methods are used. For steel quenching, it means 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 analysis, both strains due to thermal strain and strains due to phase changes have to be taken into account.[1] Physical and mechanical materials properties, as functions of structure and temperature, should be known in each moment during the quenching. 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 types of quenching remains unavailable. Although many attempts have been made to develop theoretical models to describe steel quenching, all the earlier work relied on simplifications that rendered the analysis unrealistic. In particular, successful description of steel quenching is not possible without a good theoretical explanation of all physical processes involved in the mathematical model. Second, the real complexities of plasticity have to be introduced into the model, but it is known that the theory of plasticity is not sufficiently developed. Moreover, change of physical and mechanical properties by temperature change have to be involved in the 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 hand, the Finite Volume Method (FVM) has been established as a very efficient way of solving heat transfer problems. Recently, FVM was used as a simple and effective tool for the solution of a large range of problems in the thermoplastic analysis.[3]

2. Temperature Field Change

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 law of heat conduction:

$$\frac{\partial(c\rho T)}{\partial t} = \mathrm{div}\lambda\mathrm{grad}T \qquad \text{(Eq 1)}$$

The heat sources that can exist during steel quenching are neglected in Eq 1. Axially symmetrical bodies, such as complex cylinders, cones, and spheres, can be described as 2-D problems in cylindrical coordinates r, z, and $\phi = 1$.

To solve Eq 1, the finite volume scheme is used. The time domain is divided into a number of discrete time steps, Δt, whereas the space domain is divided into a number of rectangular cells. Each cell is bounded by four faces with areas $S_{i(j,j+n)}$ and $S_{(i,i+n)j}$, ($i = 1,2 \ldots i_{max}$; $j = 1,2 \ldots j_{max}$; $n = \pm 1$), and it contains one computational nodal point at its center (Fig. 1). Linear distribution of the temperature T between neighboring points is assumed. The discretization equation system was established by integrating the differential Eq 1 over each control volume, taking into account initial and boundary conditions.

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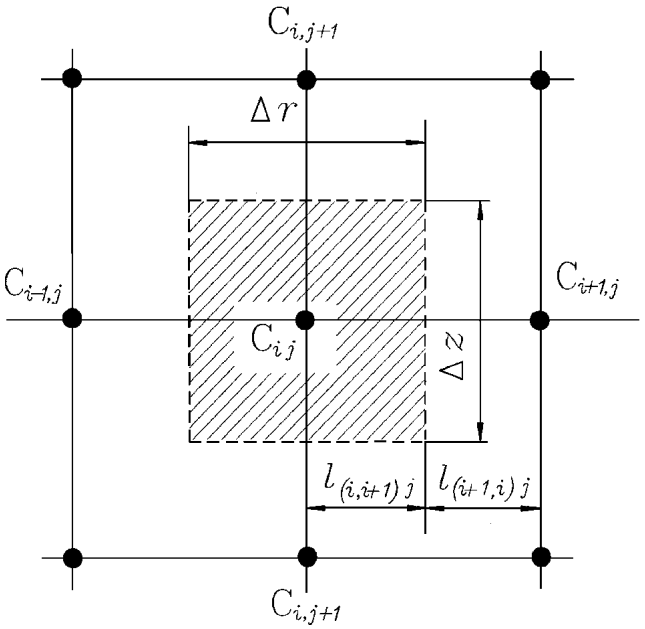

Fig. 1 Control volume for 2-D situations

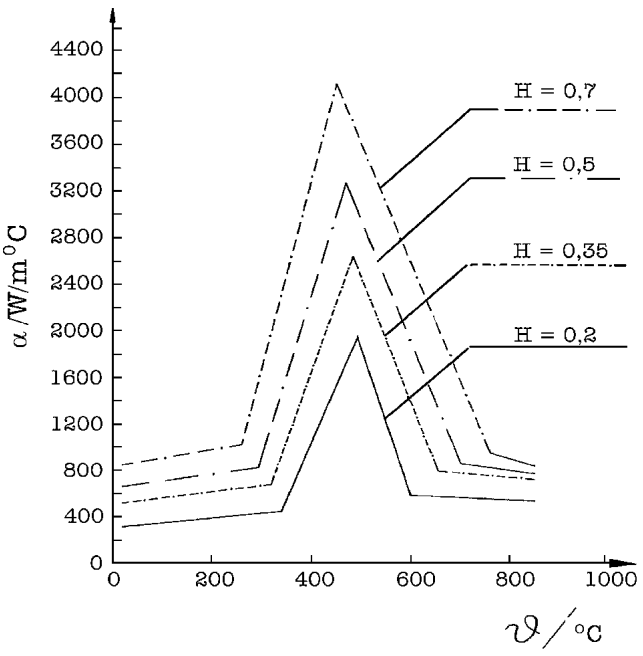

Fig. 2 Calibrated values of heat transfer coefficient α vs temperature

The discretization equation of cooling is equal[4]:

$$T_{ij}^{1}\left(\sum_{m=1}^{2} b_{(i,i+n)j} + \sum_{m=1}^{2} b_{i(j,j+n)} + b_{ij}\right) = \sum_{m}^{2}\left(b_{(i,i+n)j} T_{(i,i+n)j}^{1} + b_{i(j,j+n)} T_{i(j,j+n)}^{1}\right) + b_{ij} T_{ij}^{0}$$

$$i = 1,2 \ldots i_{max};\ j = 1,2 \ldots j_{max} \qquad n = 3 - 2\,m \qquad \text{(Eq 2)}$$

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).

The discretization system in Eq 2 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 the sum of time steps Δt and the cooling curve in each grid point of a specimen can be calculated.

Physical properties c, ρ, λ, and α have to be known. Temperature dependencies of a heat transfer coefficient and heat conductivity coefficient can be calibrated on the basis of Crafts-Lamont diagrams.[4] Calibrated values of heat transfer coefficient α versus temperature are presented in Fig. 2. For orientation, the quenchants are classified by a Grossmann's severity of cooling, i.e., H-value.

3. Stresses and Strains

The equilibrium relations in tensor notation are:

$$\sigma_{ij,i} = -F_i \qquad \sigma_{ij} = \sigma_{ji} \qquad \text{(Eq 3)}$$

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

The equilibrium and compatibility equations in thermoplastic analysis are independent of the plasticity relations. Prnadtl-Reuss plastic flow rule and Von-Mises principle hardening condition were accepted to established constitutive equation of the elastic-plastic model. In the elastic-plastic analysis the strain of transformation plasticity has been taken into account.

If it is 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:

$$\varepsilon_{ij} = \frac{1}{2G}\sigma_{ij} - \delta_{ij}\left(\frac{\mu}{E}\Theta - \alpha T - \varepsilon_{st}\right) + \varepsilon_{ij}^{pl} \qquad \text{(Eq 4)}$$

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

$$d\varepsilon_{ij}^{pl} = \frac{3}{2}\frac{S_{ij}}{\sigma_e} d\varepsilon_{pl} \qquad \sigma_e = \sqrt{\frac{3}{2} S_{ij} S_{ij}}, \quad d\varepsilon_{pl} = \sqrt{\frac{3}{2} d\varepsilon_{ij}^{pl}\, d\varepsilon_{ij}^{pl}} \qquad \text{(Eq 5)}$$

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

$$\varepsilon_{jk} = \frac{1}{2}(u_{k,j} + u_{j,k} - u_{i,j} u_{i,k}) \qquad \text{(Eq 6)}$$

To carry out such calculations it is necessary to possess 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 that relate to these unknowns in the 3-D coordinate system.

The discretization system can be established by using the finite control volume formulation. The discretized equilibrium equation of finite control volume can be established by expressing the stresses from displacements, and finally, integrating the differential equation over the control volume (Fig. 1).[3]

A system of 2N linear algebraic equations with 2N unknown displacements can be formed, where N is number of control volumes. For example, the discretized equilibrium equation in r direction for a 2-D situation is equal:

$$u_{i,j}\left(\sum_{m=1}^{2} b_{(i,i+n)j} + \sum_{m=1}^{2} b_{i(j,j+n)}\right) = \sum_{m=1}^{2}(b_{(i,i+n)j}u_{(i,i+n)j} + b_{i(j,j+n)}u_{i(j,j+n)}) + b_{i,j} \quad \text{(Eq 7)}$$

$$i = 1,2 \ldots i_{max};\ j = 1,2 \ldots j_{max} \qquad n = 3 - 2m$$

The coefficients $b_{(i,i+n)j}$, $b_{i(j,j+n)}$, $n = \pm 1$ and $b_{i,j}$ are equal:

$$b_{(i,i+n)j} = \left[(\lambda + 2G)\frac{S}{\Delta r}\right]_{(i,i+n)j} \qquad n = \pm 1 \quad \text{(Eq 8)}$$

$$b_{i(i,j+n)} = \left(G\frac{S}{\Delta z}\right)_{i(i,j+n)}$$

$$\begin{aligned} b_{i,j} = &\left[\frac{\lambda S}{\Delta z}(w_{i(j,j+1)} - w_{i(j,j-1)})\right]_{(i,i+1)j} \\ &- \left[\frac{\lambda S}{\Delta z}(w_{i(j,j+1)} - w_{i(j,j-1)})\right]_{(i,i-1)j} \\ &+ \left[\frac{GS}{\Delta r}(w_{(i,i+1)j} - {}_{(i,i-1)j})\right]_{i(j,j+1)} \\ &- \left[\frac{GS}{\Delta r}(w_{(i,i+1)j} - w_{(i,i-1)j})\right]_{i(j,j-1)} \\ &- \frac{\alpha E}{(1-2\mu)}[(ST)_{i(j,j+1)} - (ST)_{i(j,j-1)}] \end{aligned} \quad \text{(Eq 9)}$$

where $S_{(i,i+n)j}$, $S_{i(j,j+n)}$, $n = \pm 1$ are characteristic volume surfaces; $\Delta r_{(i,i+n)j}$ and $\Delta z_{i(j,j+n)}$ are characteristic finite volume dimensions; u and w are displacements in r and z direction; λ and G are Lame's coefficients.

4. Phase Transformations and Mechanical Properties

The structural transformations and mechanical properties were estimated on the basis of 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 °C (time $t_{8/5}$).[5] The hardness at grid points is estimated by the conversion of cooling time $t_{8/5}$ results to hardness by using the relation between cooling time and distance from the quenched end of the Jominy specimen shown in Fig. 3.

By involving the time $t_{8/5}$ in the mathematical model of steel hardening, the Jominy-test result could be involved in the model. Jominy values can be experimentally evaluated or calculated from elemental composition. Because 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 from only elemental composition. The grain size at the austenitizing temperature must be known for 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 from the predicted structure composition. The critical temperature of austenite decomposition could be estimated by empirical formulas.[1,6]

A phase fraction can be estimated by taking into account that steel hardness is equal:

$$\begin{aligned} HV = &((\%\ \text{ferrite})\ HV_{(F)} + (\%\ \text{pearlite})\ HV_{(P)} \\ &+ (\%\ \text{bainite})\ HV_{(B)} + (\%\ \text{martensite})\ HV_{(M)} \\ &+ (\%\ \text{austenite})\ HV_{(A)})/100 \end{aligned} \quad \text{(Eq 10)}$$

and the amount of all phases is equal unity:

$$\begin{aligned} &(\%\ \text{ferrite} + \%\ \text{pearlite} + \%\ \text{bainite} + \%\ \text{martensite} \\ &\quad + \%\ \text{austenite})/100 = 1 \end{aligned} \quad \text{(Eq 11)}$$

When the additive rule holds for the progress of transformation, and approximating continues cooling by steps in accordance with Cahn,[7] a fraction of the transformed austenite in the pearlite during the time step Δt is equal:

$$\Delta X_i \approx 4\left(\frac{\pi}{3}\right)^{\frac{1}{4}} (I_{i-1}S_{i-1})^{\frac{1}{4}} G_{i-1}^{\frac{3}{4}} \left(\ln\frac{1}{1-X_{i-1}}\right)^{\frac{3}{4}} (1 - X_{i-1})\Delta t_i \quad \text{(Eq 12)}$$

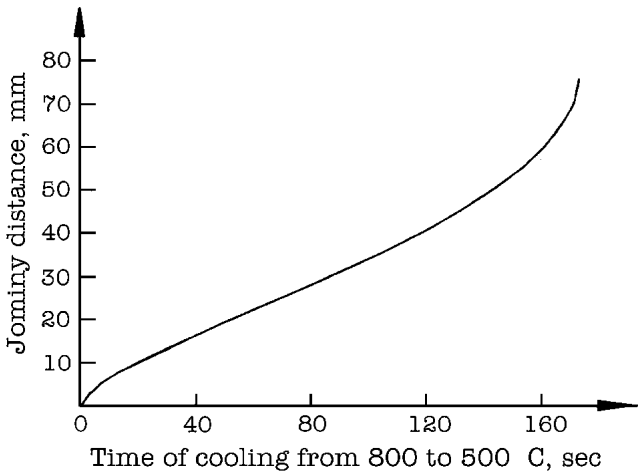

Fig. 3 Cooling time from 800 °C to 500 °C vs distance from the quenched end of Jominy specimen

Similarly, for bainite transformation:

$$\Delta X_i \approx 2S_{i-1}G_{i-1}(1 - X_{i-1})\Delta t_i \quad \text{(Eq 13)}$$

where X = is the fraction of transformed austenite, I = nucleation rate, S = nucleation site area per unit volume, and G = growth rate.

Values *I, G,* and *S* mainly depended on microstructure and temperature.

Equations 12 and 13 could be written as:

$$\Delta X_i \approx K_p f_{pl}(T, D) f_{p2}(k_{pl}, A_1, \Delta T_{pot}) \left(\ln \frac{1}{1 - X_{i-1}} \right)^{\frac{3}{4}} (1 - X_{i-1})\Delta t_i \quad \text{(Eq 14)}$$

where K_p and k_{p1} are the coefficients, D is the diffusion coefficient, and ΔT_{pot} is austenite undercooling. For austenite transformation in bainite the quantity of transformed austenite is equal:

$$\Delta X_i \approx K_b f_{b1}(T,D) f_{b2}(k_{b1} B_s \Delta T_{pot})(1 - X_{i-1})\Delta t_i \quad \text{(Eq 15)}$$

Phase hardness is dependent on the chemical composition and cooling rate. For the Jominy test, it could be written that phase hardness depends on chemical composition (*KS*) and culling rate parameter (*CRP*).

$$HV_\alpha = f_1(KS,CRP) \quad \text{(Eq 16)}$$

Phase fraction is equal:

$$\%\alpha = f_2(KS,CRP,T_A) \quad \text{(Eq 17)}$$

where T_A is the austenitizing temperature. In a task of simulation of the quenching of concrete steel, coefficients K_p, K_b, k_{p1}, and k_{b1} are calibrated by using the Jominy test results of concrete steel. For this purpose, the cooling curves of the Jominy specimen have to be known (Fig. 4).

Mechanical properties of steel during quenching directly depend on the degree of quenched steel hardening and temperature[8]. Mechanical properties R_e, K_{Ic}, *v, E,* hardening coefficient, and exponent could be estimated from HV.[8]

Mechanical property = *f* (HV Hardness, Microstructure composition, Temperature) (Eq 18)

5. Application

The mathematical model has been used for simulation of mechanical properties and residual stresses in quenched workpieces with complex form (Fig. 5). The investigation was done with the steel 530 A 36 (BS), having the elemental composition in wt.% of 0.39% C, 0.26% Si, 0.67% Mn, 1.06% Cr, 0.013% P, and 0.026% S.

Heat treatment for quenching of steel 530 A 36 was heating on 830 °C for 30 min and oil quenching. The specimen was quenched in agitated oil with the severity of quenching, i.e., Grossmann's H value equal to 0.45. Calibrated values of heat transfer coefficients for oil with an H value equal to 0.45 were used in mathematical modeling (Fig. 2). Experimentally evaluated Jominy results of investigated steel are shown in Table 1.

Figure 6 shows computed and experimentally estimated results of HRC hardness of the hardened specimen. The values of experimentally estimated hardness are converted from HV

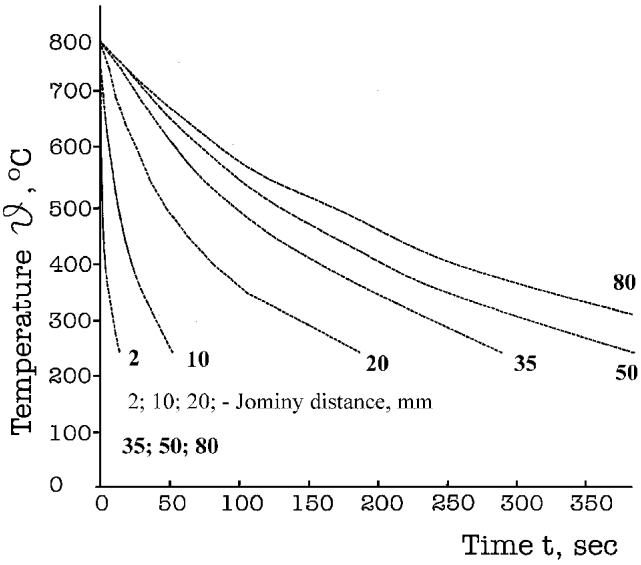

Fig. 4 Cooling curve of Jominy specimen

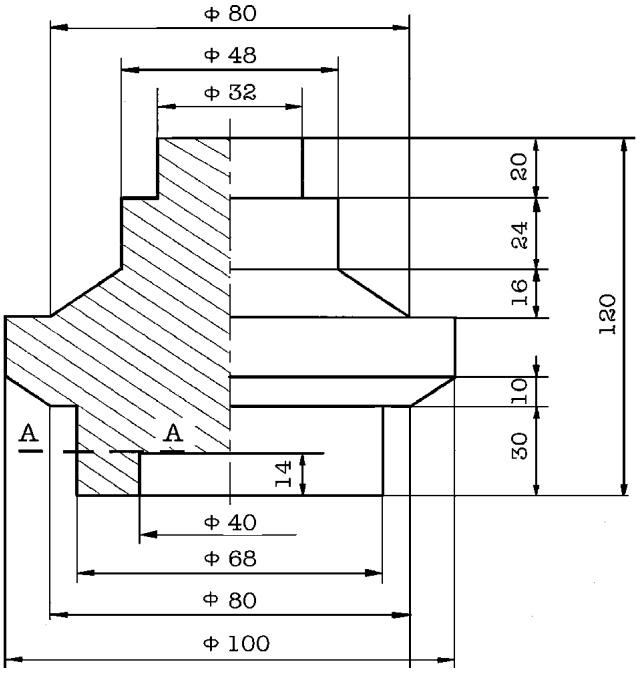

Fig. 5 Specimen

Table 1 Jominy Test Result

Distance, mm	2.5	5	7.5	10	12.5	15	20	25	30	40	50
Hardness HRC	55	54	50	45	40	36	33	32	31	26	24

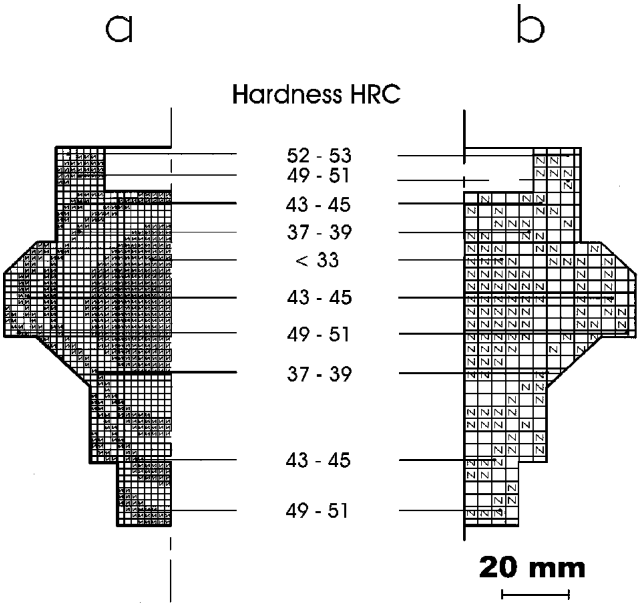

Fig. 6 Hardness distribution: (a) mathematical modeling, (b) experiment

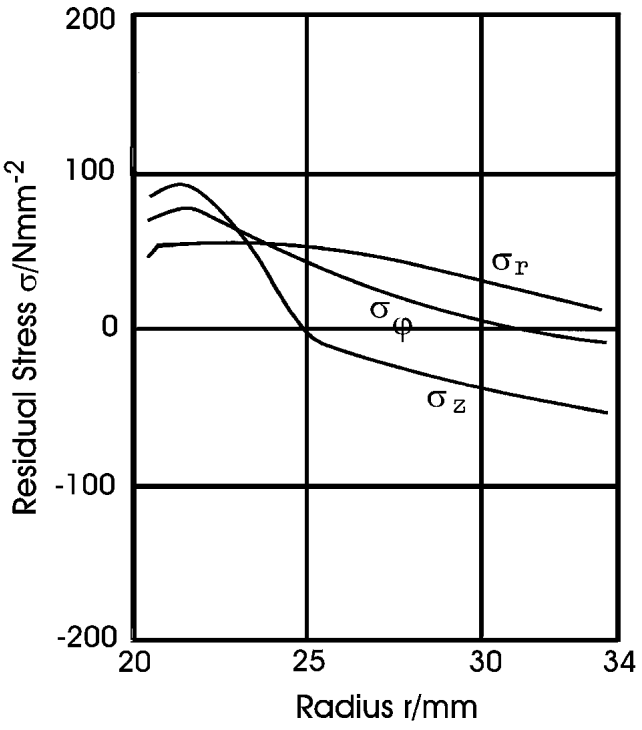

Fig. 7 Residual stress distribution in section A-A

hardness to HRC hardness. Maximum residual stresses exist in section A-A (Fig. 5). The distribution of stresses in section A-A is shown in Fig. 7.

6. Conclusion

A mathematical model of steel quenching has been developed to predict the distribution of mechanical properties and strain and residual stresses in a specimen with complex geometry. The model is based on the finite volume method and consists of numerical calculation of temperature fields in the process of cooling, numerical simulation of hardness, microstructure, and mechanical properties, and numerical simulation of stresses and strains.

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

Mathematical modeling of cooling is based on calibrated heat transfer values. Hardness in specimen points was estimated on the basis of the time of cooling from 800 °C to 500 °C, i.e., by the conversion of the mentioned specific time to hardness results. In this way the Jominy test results have been used in the mathematical model. Microstructure fraction has been estimated on the basis of chemical composition, Jominy test results, and time of cooling from 800 °C to 500 °C.

The established model has been applied in the computer simulation of hardness, residual stresses, and distortions of the quenched specimen with complex form. Comparison of the mathematical modeling results with the experiment showed that the presented model has a good performance of steel quenching simulation.

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