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Analiza občutljivosti toplotne obdelave jekel

A Sensitivity Analysis of the Heat Treatment of Steel

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Prispevek obravnava matematični model toplotne obdelave podeutektoidnih ogljikovih jekel. Pri izračunu zaostalih napetosti, ki so posledica faznih premen in temperaturnih sprememb, sta v modelu upoštevana tako kinetika faznih prehodov kakor termoelasto-plastične konstitutivne enačbe. Izdelani računalniški progam je bil preverjen na že objavljenih rezultatih. Z uporabo analize občutljivosti je ocenjena napaka v izračunanih zaostalih napetostih na temelju ocenjenih napak podatkov o lastnostih materiala.

(Ključne besede: obdelave jekel, obdelave toplotne, analize občutljivosti, modeli matematični)

This paper presents a mathematical model of the heat treatment of hypoeutectoid carbon steel. In the model, the kinetics of phase changes and a thermo-elasto-plastic constitutive relation have been applied to calculate the residual stresses resulting from phase changes and temperature variations. The computer code has been verified for internal consistency with previously published results. The sensitivity analysis has been applied to predict errors in the residual stresses from the estimated errors in the material data.

(Keywords: steel treatment, heat treatment, sensitivity analysis, mathematical models)

0 UVOD

Matematično modeliranje toplotne obdelave jekel je bilo predmet številnih raziskav v zadnjih desetletjih [10]. Te raziskave so pokazale, da se da toplotna obdelava analizirati z mehaniko kontinuov in naslednjimi predpostavkami:

- reološki model kontinua je termoelastoplastični material;
- model mora vključevati deformacije zaradi strukturnih sprememb in preoblikovalno plastičnost;
- enačba prevoda toplote mora vsebovati člen, ki popisuje toploto fazne premene;
- za popis difuzijskih faznih premen se uporablja Avramijeva enačba;
- za obravnavo austenitno-martenzitne transformacije se uporablja Koistinen-Marburgerjeva enačba;
- vse lastnosti materiala so linearne funkcije prostorninskih deležev posameznih faz.

S temi predpostavkami je proces toplotne obdelave določen kot deterministični mehanski model kontinua. S tem modelom se da ob predpostavki, da so znani podatki o mehanskih

0 INTRODUCTION

Mathematical modeling of the heat treatment of steel was intensively investigated over the last two decades [10]. It was shown that the problem of heat treatment can be analyzed by using the theory of continuum mechanics with the following assumptions:

- a continuum rheologic model is thermo-elasto-plastic;
- in the mechanical model the structural phase deformation and transformation plasticity have to be included;
- the equation of heat transfer is added to the part which represents the heat of the phase transformation;
- the Avrami equation is used for treating the kinetics of the diffusion-controlled transformation of phases;
- Koistinen-Marburger's equation is used for treating the austenite-martensite transformation;
- all the properties of the continuum are linear functions of the volume fractions of the phases.

With these assumptions, the heat-treating process is defined by a deterministic mechanical model of continuum. Using this model, and provided that the data of the mechanical properties and bound-

lastnostih in ob znanih robnih pogojih izračunati zaostale napetosti.

Poglavitni namen tega prispevka je oceniti napako izračunanih zaostalih napetosti na podlagi ocene napak vhodnih podatkov o materialu. V ta namen je bil izdelan matematični model toplotne obdelave. Na temelju modela je bil izdelan računalniški program, ki izračuna razvoj temperature, strukturnih sprememb in zaostalih napetosti pri ohlajanju neskončnega valja, izdelanega iz podeutektoidnega ogljikovega jekla. Računalniški program je bil primerjalno testiran z rezultati objavljenimi v literaturi. V nadaljevanju so bili izračunani koeficienti občutljivosti za valje premera 10 mm, 30 mm in 50 mm izdelanih, iz izbranega materiala. Na podlagi koeficientov občutljivosti smo ocenili vplivnost vhodnih podatkov in nadalje, na podlagi ocenjenih napak vhodnih podatkov smo ocenili še napako v izračunu zaostalih napetosti.

1 MATEMATIČNI MODEL

Matematični model toplotne obdelave mora vključevati izračun temperature, strukture in napetosti. V tem poglavju podajamo pregled osnovnih enačb, ki so vključene v model.

1.1 Opis materiala

Jeklo, ki je izpostavljeno toplotni obdelavi, obravnavamo kot zmes N sestavin. Te so: austenit, ferit, perlit, bainit in martenzit. Če je ξ_k prostorninski delež k-te sestavine, potem velja:

$$\sum_{k=1}^{N} \xi_k = 1 \tag{1}$$

Če je w_k masni delež k-te sestavine, potem velja podobno:

$$\sum_{k=1}^{N} w_k = 1 \tag{2}$$

Vsaka sestavina zmesi ima gostoto ρ_k. Če je ρ gostota zmesi, potem sta prostorninski in masni delež k-te sestavine povezana na naslednji način:

$$w_k = \frac{\rho_k}{\rho} \xi_k \tag{3}$$

Pri jeklu so razlike med gostotami posameznih sestavin majhne, zato velja ocena $w_k \approx \xi_k$. Iz (1) do (3) se da izpeljati naslednji zvezi, ki ju bomo uporabili v nadaljevanju:

$$\rho = \sum_{k=1}^{N} \rho_k \xi_k \tag{4}$$

$$\frac{1}{\rho} = \sum_{k=1}^{N} \frac{w_k}{\rho_k} \tag{5}$$

ary conditions are known, the residual stresses in a treated element can be calculated.

The main aim of this paper was to estimate the error in the calculated residual stresses from the estimated error in the inputed material data. In order to do this a mathematical model of the heat treatment was developed. This model was converted to a computer program which performed the calculation of the thermal and structural evaluations and the residual stresses during the cooling of an infinitely long cylinder made of hypoeutectoid carbon steel. The computer code was verified for internal consistency with previously published results. Next, the sensitivity coefficients of the selected material data were calculated for cylinders of 10 mm, 30 mm and 50 mm diameter. On the basis of the sensitivity coefficients we estimated the importance of the input data and, in addition, using the estimated errors of the material data we determined the error in the calculated residual stresses.

1 MATHEMATICAL MODEL

A consistent mathematical model of heat treatment must include thermal, structural and stress calculations. In this section we shall review the essential equations which were used in the model.

1.1 Material description

The steel used in the heat-treatment process is considered to be a mixture of N constituents: austenite, ferrite, pearlite, bainite and martensite. If ξ_k is the volume fraction of the kth constituent then:

$$\sum_{k=1}^{N} \xi_k = 1 \tag{1}$$

Similarly, if w_k is the mass fraction of the kth constituent then:

$$\sum_{k=1}^{N} w_k = 1 \tag{2}$$

Each constituent of the mixture has a density ρ_k. If ρ is the mixture density, then the volume fraction and the mass of the kth constituent are connected by:

$$w_k = \frac{\rho_k}{\rho} \xi_k \tag{3}$$

In the case of steel, the differences between the densities of the constituents are small, so in this case we have $w_k \approx \xi_k$. On the basis of (1) to (3), the following relations, which will be used later, can be derived:

$$\rho = \sum_{k=1}^{N} \rho_k \xi_k \tag{4}$$

$$\frac{1}{\rho} = \sum_{k=1}^{N} \frac{w_k}{\rho_k} \tag{5}$$

1.2 Elastičnost

Če predpostavimo, da je material izotropen, potem so elastične deformacije ε_{ij}^{e} podane z:

$$\varepsilon_{ij}^{e} = \frac{1}{E}\left[(1+\nu)\sigma_{ij} - \nu\sigma_{mm}\delta_{ij}\right] + \alpha\vartheta\delta_{ij} + \left(\sum_{k=1}^{N}\gamma_k\xi_k\right)\delta_{ij} \quad (6).$$

Pri tem so σ_{ij} napetostni tenzor, E, ν in α Youngov modul, Poissonovo razmerje in koeficient termičnega raztezanja, γ_k pa dilatacijski koeficient k-te sestavine. Nadalje predpostavimo, da so ν in γ_k konstante, E in α pa linearni funkciji prostorninskih deležev:

$$E = \sum_{k=1}^{N} E_k(\vartheta)\,\xi_k \quad (7)$$

$$\alpha = \sum_{k=1}^{N} \alpha_k\,\xi_k \quad (8),$$

pri čemer je $E(\vartheta)$ temperaturno odvisni Youngov modul k-te sestavine in α_k njen razteznostni koeficient, za katerega predpostavimo, da je nespremenljiv.

Dilatacijski koeficient γ_k lahko izračunamo takole: če so deformacije majhne, potem po zakonu ohranitve mase in (4) dobimo:

$$\varepsilon_v = 1 - \frac{\rho}{\rho_0} = \sum_{k=1}^{N}\frac{\rho_k - \rho_0}{\rho_0}\xi_k \quad (9),$$

pri čemer je ε_v prostorninska deformacija in ρ_0 gostota zmesi v referenčnem stanju. S primerjavo te enačbe in (6) dobimo za $\sigma_{ij} = 0$ in $\vartheta = 0$:

$$\gamma_k = \frac{1}{3}\frac{\rho_0 - \rho_k}{\rho_0} \quad (10).$$

1.3 Plastičnost

Prirastek plastičnih deformacij $d\varepsilon_{ij}^{p}$ izračunamo z uporabo klasične teorije plastičnosti in Missesovega kriterija tečenja:

$$F = s_{ij}s_{ij} - \frac{2}{3}\sigma_f^2 \quad (11)$$

$$d\varepsilon_{ij}^{p} = d\Lambda^{p} s_{ij} \quad (12),$$

pri čemer je s_{ij} deviatorični napetostni tenzor, definiran kot:

$$s_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{mm}\delta_{ij} \quad (13)$$

in σ_f napetost tečenja. Pogoj $F < 0$ pomeni, da ni plastičnega tečenja, pogoj $F = 0$ pa, da je. Če združimo (11) in (12), dobimo:

$$d\Lambda^{p} = \frac{3}{2}\frac{d\varepsilon^{p}}{\sigma_f} \quad (14)$$

pri čemer je $d\varepsilon^{p}$ dejanski prirastek plastičnih deformacij, podan z:

1.2 Elasticity

If we assume that a material is isotropic, then the elastic strain ε_{ij}^{e} is given by:

Here σ_{ij} is the stress tensor, E, ν and α are theYoung's modulus, Poisson's ratio and thermal expansion coefficient, respectively, and γ_k is the dilatation coefficient of the kth constituent. We assume that ν and γ_k are constants. E and α are taken as linear functions of the volume fractions of the constituents:

where $E(\vartheta)$ is the temperature-dependent Young's modulus of the kth constituent and α_k is its thermal expansion coefficient, which is assumed to be constant.

We shall now describe a method for calculating the dilatation coefficients γ_k. If deformations in the material are small, then from the conservation of mass and equation (4) we obtain:

where ε_v is the volume deformation and ρ_0 is the mixture density in a reference state. By comparing this equation with equation (6) at $\sigma_{ij} = 0$ and $\vartheta = 0$ we obtain:

1.3 Plasticity

The plastic strain increment $d\varepsilon_{ij}^{p}$ is calculated using the classical theory of plasticity with the Misses yield criterion and the associated flow rule. Thus:

where s_{ij} are the components of the deviatoriv stress tensor given by:

and σ_f is the flow stress. The condition $F < 0$ means that there is no plastic flow and $F = 0$ means that plastic flow takes place. Combining of (11) and (12) gives:

where $d\varepsilon^{p}$ is the effective plastic strain increment given by:

$$d\varepsilon^p = \sqrt{\frac{2}{3} d\varepsilon_{ij}^p d\varepsilon_{ij}^p} \tag{15}$$

Predpostavimo, da je napetost tečenja podana z linearnim zakonom utrjevanja:

We assume that the flow stress is given by the linear hardening rule:

$$\sigma_f = \sigma_Y + H\varepsilon^p \tag{16},$$

pri čemer je σ_Y napetost tečenja in H koeficient utrjevanja. Nadalje predpostavimo, da sta napetost tečenja in koeficient utrjevanja linearni funkciji prostorninskih deležev posameznih sestavin:

where σ_Y is the yield stress and H is the strain-hardening coefficient. In addition, we assume that the yield stress and the strain-hardening coefficient are linear functions of the volume fractions of constituents:

$$\sigma_Y = \sum_{k=1}^{N} \sigma_{Y,k}(\vartheta)\, \xi_k \tag{17}$$

$$H = \sum_{k=1}^{N} H_k(\vartheta)\, \xi_k \tag{18}.$$

Pri tem sta $\sigma_{Y,k}$ in H_k napetost tečenja in koeficient utrjevanja k-te sestavine.

Here, $\sigma_{Y,k}$ and H_k correspond to the yield stress and the strain-hardening coefficient of the kth constituent, respectively.

1.4 Preoblikovalna plastičnost

Za izračun prirastka preoblikovalne plastičnosti $d\varepsilon_{ij}^{tp}$ uporabimo model, ki so ga predlagali v [11] in [15]:

1.4 Transformation Plasticity

For the calculation of the transformation plasticity strain increment $d\varepsilon_{ij}^{tp}$ we applied the model proposed in [11] and [15]:

$$d\varepsilon_{ij}^{tp} = d\Lambda^{tp} s_{ij} \tag{19},$$

pri čemer je:

where

$$d\Lambda^{tp} = 3\sum_{k=2}^{N} K_k \left(1-\xi_k\right) d\xi_k \tag{20}$$

in K_k konstante, ki jih je treba določiti s preskusi.

and K_k are constants which must be determined experimentally.

1.5 Prevod toplote

Temperaturno polje dobimo z rešitvijo enačbe prevoda toplote:

1.5 Heat Conduction

The temperature field is calculated by solving the basic equation of heat conduction:

$$c\frac{\partial \vartheta}{\partial t} = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial \vartheta}{\partial x_i}\right) + \sum_{k=2}^{N} l_k \xi_k \tag{21},$$

pri čemer so t čas, ϑ temperatura, c specifična toplota, λ koeficient prevoda toplote in l_k latentne toplote premen.

Temperaturno odvisna c in λ vzamemo kot linearni funkciji prostorninskih deležev sestavin:

where t is time, ϑ is the temperature, c is the heat capacity, λ is the coefficient of thermal conductivity and l_k are the enthalpies of transformation.

Both c and λ are temperature dependent and are taken as linear functions of the volume fractions of the constituents:

$$c = \sum_{k=1}^{N} c_k(\vartheta)\, \xi_k \tag{22}$$

$$\lambda = \sum_{k=1}^{N} \lambda_k(\vartheta)\, \xi_k \tag{23},$$

pri čemer sta $c_k(\vartheta)$ in $\lambda_k(\vartheta)$ specifična toplota in toplotna prevodnost sestavine k. Enačbo (21) rešujemo skupaj s konvekcijskim robnim pogojem:

and $c_k(\vartheta)$ and $\lambda_k(\vartheta)$ the heat capacity and the thermal conductivity for phase k. Equation (21) is solved together with convection, boundary condition:

$$-\lambda \frac{\partial \vartheta}{\partial n} = h\left(\vartheta - \vartheta_e\right) \tag{24},$$

pri čemer je h konvekcijski koeficient, ki je lahko temperaturno odvisen in ϑ_e temperatura okolice.

where h is the convection heat-transfer coefficient, which may be temperature dependent and ϑ_e is the environmental temperature.

1.6 Fazne premene

Opazujmo fazni prehod faze m v fazo n. V ta namen prepišimo (1) v obliko:

1.6 Phase Transformations

We can consider the phase transformation from, say, phase m to phase n. For this purpose we write equation (1) as:

$$\xi_m + \xi_n = 1 - \sum_{k \neq m,n} \xi_k \tag{25}$$

in uvedimo novo spremenljivko ζ, definirano kot:

and then introduce a new variable ζ defined by:

$$\zeta = \frac{\xi_n}{1 - \sum_{k \neq m,n} \xi_k} \tag{26},$$

ki jo bomo uporabili za opis napredovanja premene. Pri izotermnih pogojih se da heterogena premena opisati z Avramijevo enačbo ([5],[6] in [16]):

which will be used to describe the extent of the transformation. Under isothermal conditions a heterogeneous solid-state transformation can be described by the Avrami equation ([5],[6] and [16]):

$$\zeta = 1 - \exp\left[-(\beta t)^n\right] \tag{27},$$

pri čemer je

where

$$\beta(\vartheta) = K_0 (\vartheta_E - \vartheta)^n \exp\left[-\frac{Q}{T}\right] \tag{28}.$$

K_0 in Q sta konstanti, n je Avramijev eksponent, ki je odvisen od geometrijske oblike rastočih kristalnih zrn in je temperaturno neodvisen [6], T je absolutna temperatura, ϑ_E pa ravnotežna temperatura premene. Za neizotermne pogoje se da Avramijeva enačba zapisati v obliki:

K_0 and Q are constants, n is the Avrami exponent, which is dependent on grain growth geometry and can be taken as temperature independent [6], T is the absolute temperature, and ϑ_E is the equilibrium temperature of the transformation. For nonisothermal conditions the Avrami equation can be written in the form:

$$\frac{d\zeta}{dt} = n\beta(\vartheta)(1-\zeta)\left[-\ln(1-\zeta)\right]^{\frac{n-1}{n}} \tag{29},$$

ki jo dobimo, če iz (27) izločimo čas t.

which is obtained by eliminating t from (27).

Ko je n konstanta, se da K_0 in Q dobiti iz diagramov TTT takole: čas t_0, ki je potreben za premeno ζ_0 pri dani temperaturi T, je iz (27):

When n is constant, K_0 and Q can be determined from TTT diagrams in the following way. The time t_0 for a fixed amount of transformation ζ_0 at a given temperature T is, from (27):

$$t_0 = t_0(\vartheta) = \frac{K_0 e^{\frac{Q}{T}}}{(\vartheta_E - \vartheta)^n}\left[-\ln(1-\zeta_0)\right]^{\frac{1}{n}} \tag{30}.$$

Če sta (t_m, ϑ_m) koordinati ekstrema na krivulji TTT, potem je v tej točki $dt/d\vartheta = 0$. Iz tega pogoja in (30) izhaja:

If (t_m, ϑ_m) are coordinates of the nose in the TTT curve then $dt/d\vartheta = 0$ at this point. From these conditions and (30) it follows that:

$$Q = \frac{n T_m^2}{\vartheta_E - \vartheta_m} \tag{31}.$$

Ko poznamo Q, lahko iz (30) izračunamo K_0:

By knowing Q we can calculate K_0:

$$K_0 = t_m (\vartheta_E - \vartheta_m)^n e^{-\frac{Q}{T_m}} \left[\ln(1-\zeta_0)\right]^{\frac{1}{n}} \tag{32}.$$

Martenzitna premena je odvisna le od temperature, zato ima v tem primeru kinetični zakon obliko $\zeta = f(\vartheta)$. Iz te enačbe je prirastek premene $d\zeta = f'(\vartheta)d\vartheta$.

A martensitic transformation depends only on temperature, therefore the kinetic law is, in this case, given by $\zeta = f(\vartheta)$. From this equation the increment of

Iz osnovnega kinetičnega zakona lahko izrazimo ϑ kot funkcijo ζ, zato je $d\zeta = g(\zeta)d\vartheta$. Ko je premena končana, tj. ko je $\zeta = 1$, mora biti $g(\zeta) = 0$. Najpreprostejša funkcija, ki ustreza temu pogoju, je linearna, torej:

transformation is $d\zeta = f'(\vartheta)d\vartheta$. From the kinetic law we can express ϑ as a function of ζ, hence $d\zeta = g(\zeta)d\vartheta$. When the transformation is completed i.e. when $\zeta = 1$, we must have $g(\zeta) = 0$. The simplest equation compatible with this requirement is linear, namely:

$$d\zeta = k_M \left(1-\zeta\right) d\vartheta \tag{33}.$$

Z integracijo dobimo:

By integrating this equation we obtain:

$$\zeta = 1-\exp\left[-k_M \left(\vartheta - M_s\right)\right] \tag{34},$$

pri čemer je M_s temperatura, pri kateri se začne martenzitna premena. Enačba (34) je identična Koinstinen-Marburger empirični enačbi [10]. Za večino jekel ima konstanta k_M vrednost 0,011.

where M_s is the martensitic starting temperature. Equation (34) is identical with the Koinstinen-Marburger empirical formula [10]. The constant k_M is equal to 0.011 in most steels.

2 LASTNOSTI MATERIALA

V tej raziskavi smo za material izbrali podeutektoidno ogljikovo jeklo, ker je za ta material v literaturi dostopnih dovolj podatkov, s katerimi lahko zgradimo analitični model materiala. V nadaljevanju bomo uporabili oznake *A,B,M,P* in *W* za austenit, bainit, martenzit, perlit in cementit. Simbole *C*, *Si* in *Mn* bomo uporabili za masne deleže ogljika, silicija in mangana v jeklu.

2.1 Youngov modul in Poissonovo število

Za ogljikova jekla se da Youngov modul perlita izračunati po naslednjem obrazcu:

$$E_P = 209,3 - 0,076\,\vartheta \pm 1,62 \quad \text{GPa} \tag{35}.$$

Ta obrazec je dobljen na podlagi regresijske analize podatkov, ki jih je podal [7]. Predpostavljamo, da ta obrazec velja prav tako za bainit in martenzit. Obrazec, ki podaja Youngov modulu austenita, smo dobili iz podatkov, ki jih navaja [22] in ima obliko:

$$E_A = 200,2 - 0,08\,\vartheta \pm 0,32 \ \text{GPa} \tag{36}.$$

Predpostavljamo, da ima Poissonovo število vrednost 0,3 za vse sestavine.

2.2 Razteznostni koeficient

V literaturi ni zaslediti enotnih podatkov za vrednost razteznostnih koeficientov, zato smo vzeli naslednje vrednosti [10]:

2 MATERIAL PROPERTIES

As a target material in this investigation we chose hypoeutectoid carbon steel because there were enough data available in the literature to construct a material model as well as the analytical formulas. In the following we use the indices *A,B,M,P* and *W* for austenite, bainite, martensite, pearlite and cementite, respectively. We will also use the symbols *C*, *Si* and *Mn* to denote the weight percent of carbon, silicon and manganese in the steel.

2.1 Young's Modulus and Poisson's Ratio

For carbon steel the Young's modulus of pearlite is calculated by:

This formula was obtained on the basis of a regression analysis from the data [7]. We assume that the same formula holds for bainite and martensite. The formula for the Young's modulus of austenite was obtained from data reported by [22] and has the form:

The Poisson's number is assumed to be constant and is equal to 0.3 for all constituents.

2.2 Coefficient of Expansion

There is no single value in the literature for the expansion coefficient of the different phases so in the present model we adopted the following values [10]:

$$\begin{aligned} \alpha_A &= 22\cdot 10^6 \ \ \mathrm{K}^{-1} \\ \alpha_B &= 13\cdot 10^6 \ \ \mathrm{K}^{-1} \\ \alpha_M &= 12\cdot 10^6 \ \ \mathrm{K}^{-1} \\ \alpha_P &= 14\cdot 10^6 \ \ \mathrm{K}^{-1} \end{aligned} \tag{37}.$$

Iz podatkov v literaturi ocenjujemo, da so podane vrednosti znotraj območja $\pm 1 \cdot 10^{-6}\ \mathrm{K}^{-1}$.

From the data published in the literature we conclude that all the above values are within the range $\pm 1 \cdot 10^{-6}\ \mathrm{K}^{-1}$.

2.3 Preoblikovalna deformacija

Večina znanih del uporablja za dilatacijske koeficiente eksperimentalne vrednosti iz [10]. V tem delu bomo dilatacijske koeficiente izračunali na temelju kristalografskih podatkov iz preglednice 1 in (10). Iz kristalografskih podatkov izračunamo linearizirane gostote sestavin jekla:

2.3 Transformation Strain

Most previous studies used experimental values for the dilatation coefficients [10]. We have chosen to calculate these values on the basis of the crystallographic data in table 1 and equation (10). From crystallographic data the following linearised densities of the steel constituents are obtained:

$$\begin{aligned} \rho_A &= 8156 - 216\,C \ \ \mathrm{kg/m^3} \\ \rho_B &= 7897 \ \ \mathrm{kg/m^3} \\ \rho_M &= 7676 \ \ \mathrm{kg/m^3} \\ \rho_F &= 7897 - 248\,C \ \ \mathrm{kg/m^3} \end{aligned} \qquad (38).$$

Preglednica 1. *Kristalografski podatki*
Table 1. *Crystallographic data*

Faza Phase	Tip Type	Fe	C	Lattice parameters [Å]	Vir Source
Austenit Austenite	fcc	4	-	a = 3,5735 + 0,0316C	[19]
Cementit Cementite	ort	12	3	a = 4,5234 b = 5,0883 c = 6,7426	[4]
Ferit Ferrite	bcc	2	0	a = 2,8664	[4]
Martenzit Martensite	bct	2	-	a = 2,8664 – 0,013C c = 2,8664 + 0,116C	[4]

Iz (4) je gostota perlita:

From (4) we have for the pearlite density:

$$\frac{1}{\rho_P} = \frac{0{,}12}{\rho_W} + \frac{0{,}88}{\rho_F} \qquad (39),$$

iz katere dobimo, če vstavimo vrednosti iz (38):

which gives, by substituting values from (38), the following value:

$$\rho_P = 7861 \ \ \mathrm{kg/m^3} \qquad (40).$$

Podobno dobimo gostoto zmesi ferita in perlita:

For the ferrite-pearlite mixture we then obtain, by a similar procedure, the result:

$$\rho_{P+F} = 7897 - 45\,C \ \ \mathrm{kg/m^3} \qquad (41).$$

Če vzamemo za referenčno strukturo jekla zmes ferita in perlita, dobimo na podlagi (10):

If we take the mixture of ferite-perlite as a steel reference structure then from (10) we obtain:

$$\begin{aligned} \gamma_A &= -0{,}0109 + 0{,}0072\,C \\ \gamma_M &= 0{,}0086\,C \end{aligned} \qquad (42).$$

Prav tako predpostavimo, da je $\gamma_B = 0$.

We also assume that $\gamma_B = 0$.

2.4 Meja tečenja in koeficient utrjevanja

Iz podatkov, ki sta jih objavila [12] in [10], dobimo naslednje obrazce za mejo plastičnega tečenja:

$$\begin{aligned}\sigma_{Y,A} &= 123 - 0{,}1\vartheta - 0{,}01C\vartheta \pm 1{,}3 \ \text{MPa}\\ \sigma_{Y,P} &= 434 - 0{,}64\vartheta + 0{,}77C\vartheta \pm 34{,}4 \ \text{MPa}\\ \sigma_{Y,B} &= 491 + 757C - 1{,}02C\vartheta \pm 26{,}1 \ \text{MPa}\\ \sigma_{Y,M} &= 445 + 1375C \pm 30{,}4 \ \text{MPa}\end{aligned} \tag{43}$$

in koeficient plastičnega utrjevanja:

$$\begin{aligned}H_A &= 45{,}3 - 0{,}04\vartheta \pm 0{,}63\times 10^2 \ \text{MPa}\\ H_B &= 5{,}88 + 226{,}2C\vartheta \pm 19{,}7\times 10^2 \ \text{MPa}\\ H_F &= 29{,}5 + 0{,}33C\vartheta \pm 41{,}7\times 10^2 \ \text{MPa}\\ H_M &= 179 + 1{,}3C\vartheta \pm 29{,}9\times 10^2 \ \text{MPa}\end{aligned} \tag{44}.$$

2.5 Koeficienti preoblikovalne plastičnosti

Na temelju poskusov, opisanih v [18], smo vzeli naslednje vrednosti konstant K_k:

$$\begin{aligned}K_B &= 4{,}18\cdot 10^{-5} \ \text{MPa}^{-1}\\ K_M &= 5{,}08\cdot 10^{-5} \ \text{MPa}^{-1}\\ K_P &= 4{,}18\cdot 10^{-5} \ \text{MPa}^{-1}\end{aligned} \tag{45}.$$

2.6 Specifična toplota

Podatki za regresijsko analizo specifične toplote so vzeti iz [9]. Iz teh podatkov je specifična toplota perlita:

$$c_p^P = 3{,}76 + 0{,}3C + 6{,}2 10^{-6}\vartheta^2 \pm 0{,}15 \ \ \text{MJ/m}^3\text{K} \tag{46}.$$

Predpostavimo, da ta obrazec velja tudi za bainit in martenzit. Za specifično toploto austenita smo uporabili obrazec:

$$c_p^A = 4{,}152 + 8{,}410^{-4}\vartheta \ \ \text{MJ/m}^3\text{K} \tag{47},$$

dobili smo ga iz podatkov v [22].

2.7 Toplotna prevodnost

Regresijsko formulo za toplotno prevodnost perlita smo dobili iz podatkov, objavljenih v [3] in [8]:

$$\lambda^P = 66{,}2 - 37{,}9C - 0{,}049\vartheta \pm 1{,}74 \ \ \text{W/mK} \tag{48}.$$

Predpostavimo, da ta obrazec velja tudi za bainit. Za martenzit smo vzeli vrednost $\lambda_M = 30 \pm 5$ W/mK, kakor jo predlaga [10]. Iz podatkov, objavljenih v [22], smo dobili naslednji obrazec za izračun toplotne prevodnosti austenita:

$$\lambda_A = 15 + 0{,}01\vartheta \ \ \text{W/mK} \tag{49}.$$

2.4 Yield Strength and Strain-Hardening Coefficient

From the data published by [12] and [10] we derive the following formulas for the yield stresses:

$$\begin{aligned}\sigma_{Y,A} &= 123 - 0{,}1\vartheta - 0{,}01C\vartheta \pm 1{,}3 \ \text{MPa}\\ \sigma_{Y,P} &= 434 - 0{,}64\vartheta + 0{,}77C\vartheta \pm 34{,}4 \ \text{MPa}\\ \sigma_{Y,B} &= 491 + 757C - 1{,}02C\vartheta \pm 26{,}1 \ \text{MPa}\\ \sigma_{Y,M} &= 445 + 1375C \pm 30{,}4 \ \text{MPa}\end{aligned} \tag{43}$$

and the coefficient of strain hardening:

$$\begin{aligned}H_A &= 45{,}3 - 0{,}04\vartheta \pm 0{,}63\times 10^2 \ \text{MPa}\\ H_B &= 5{,}88 + 226{,}2C\vartheta \pm 19{,}7\times 10^2 \ \text{MPa}\\ H_F &= 29{,}5 + 0{,}33C\vartheta \pm 41{,}7\times 10^2 \ \text{MPa}\\ H_M &= 179 + 1{,}3C\vartheta \pm 29{,}9\times 10^2 \ \text{MPa}\end{aligned} \tag{44}.$$

2.5 Transformation Plasticity Coefficient

From the experimental work of [18] the following values for the constant K_k were adopted:

$$\begin{aligned}K_B &= 4{,}18\cdot 10^{-5} \ \text{MPa}^{-1}\\ K_M &= 5{,}08\cdot 10^{-5} \ \text{MPa}^{-1}\\ K_P &= 4{,}18\cdot 10^{-5} \ \text{MPa}^{-1}\end{aligned} \tag{45}.$$

2.6 Specific Heat Capacity

The data for the regression analysis of the specific heat capacity were taken from [9]. From this we obtain the following formula:

$$c_p^P = 3{,}76 + 0{,}3C + 6{,}2 10^{-6}\vartheta^2 \pm 0{,}15 \ \ \text{MJ/m}^3\text{K} \tag{46}.$$

We take this formula to be valid also for bainite and martensite. For the austenite heat capacity we use the formula:

$$c_p^A = 4{,}152 + 8{,}410^{-4}\vartheta \ \ \text{MJ/m}^3\text{K} \tag{47},$$

which was obtained from data published in [22].

2.7 Thermal Conductivity

The regression formula for thermal conductivity was obtained from published data in [3] and [8]:

$$\lambda^P = 66{,}2 - 37{,}9C - 0{,}049\vartheta \pm 1{,}74 \ \ \text{W/mK} \tag{48}.$$

We assume that the above formula is also valid for bainite. For martensite we take the thermal conductivity to be $\lambda_M = 30 \pm 5$ W/mK, as suggested by [10]. From the data of [22] we obtain the following formula for the thermal conductivity of austenite:

$$\lambda_A = 15 + 0{,}01\vartheta \ \ \text{W/mK} \tag{49}.$$

2.8 Fazne temperature

Za izračun ravnotežnih temperatur, ki se uporabljajo v (28), smo uporabili naslednje empirične obrazce:

2.8 Transformation temperatures

For the calculation of the equilibrium temperatures which are used in (28) we chose the following empirical formulae:

$$\begin{aligned} A_1 &= 723 - 10,7\,Mn + 29,1\,Si \pm 10 \ {}^0\mathrm{C} \\ A_2 &= 910 - 203C + 44,7\,Si \pm 10 \ {}^0\mathrm{C} \\ B_s &= 830 - 270\,C - 90\,Mn \pm 25 \ {}^0\mathrm{C} \\ M_s &= 539 - 423\,C - 30,4\,Mn \pm 25 \ {}^0\mathrm{C} \end{aligned} \qquad (50).$$

Obrazce za A_1, A_3 in M_s je podal [1], temperaturo začetka tvorjenja bainita B_s pa [21].

The formulae for A_1, A_3 and M_s were given by [1], and for bainite the start temperature B_s was given by [21]

3 POSTOPEK REŠEVANJA

Opisani model je bil uveden v računalniški program, ki omogoča izračun temperature, strukture in zaostalih napetosti pri hlajenju neskončnega valja, izdelanega iz podeutektoidnega jekla. Temperaturno polje se računa na temelju implicitne metode končnih razlik, napetosti pa z metodo zaporednih približkov, ki jo podaja [17].
Vhodni podatki so:
- premer valja
- kemična sestava jekla
- začetna in končna temperatura procesa ohlajanja
- konvekcijski koeficient
- koordinate ekstremnih točk na diagramu TTT

Izhodni podatki so:
- porazdelitev zaostalih napetosti in struktur
- temperaturni in napetostni potek v osi in na površini valja

3 SOLUTION METHOD

The described model was converted into a computer program which performed the calculation of thermal and structural evaluations and the internal stresses during cooling of an infinitely long cylinder made from hypoeutectoid carbon steel. The temperature field was calculated using the implicit finite-difference method and the stress evaluation wasbased on the successive approximation method described by [17].
The input data for the program are:
- cylinder diameter,
- chemical composition of the steel,
- process start and end temperature,
- heat convection coefficient,
- coordinates of the extreme point of the TTT curves.

The output of the program is:
- residual stress and structure distribution,
- temperature-time and axial stress-time evaluation on the surface and centere of the cylinder.

4 PRESKUS MODELA

Kot prvi primer smo obravnavali valj s premerom 60 mm, izdelan iz 0,43% ogljikovega jekla, gašenega v vodi s temperature 870°C. Ta primer je teoretično in eksperimentalno obdelan v [13] in [14] in prav tako teoretično v [20].

Iz objavljenih podatkov smo ocenili, da mora biti koeficient prestopa toplote blizu 25 kW/m^{2}K. Omenimo, da tudi s tako visokim konvekcijskim koeficientom nismo dobili take hitrosti ohlajanja osi valja, kakor jo navaja [13]. Kljub temu pa so izračunane zaostale napetosti v skladu z eksperimentalnimi vrednostmi, kakor se vidi s slike 1.

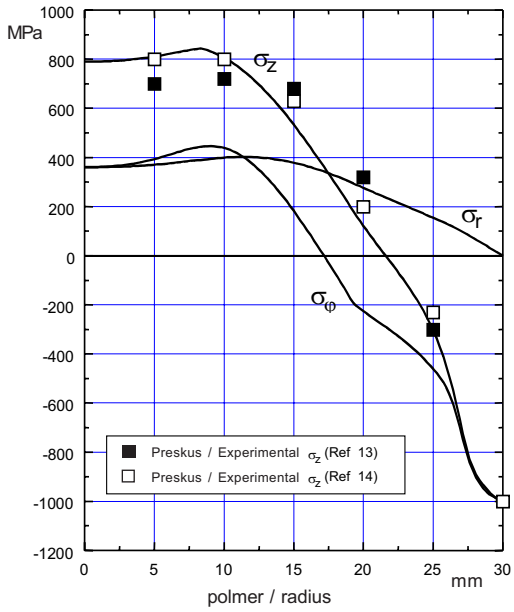
Kot drug primer so obravnavali valje s premeri 10 mm, 30 mm, 50 mm in 100 mm izdelane iz 0,44% ogljikovega jekla. Porazdelitev zaostalih napetosti za take valje eksperimentalno obravnava [2], teoretično pa [23]. Vsi valji so gašeni v vodi na 20 °C s temperaturo 850 °C. Vrednosti konvekcijskega koeficienta smo vzeli med 3200 W/m^{2}K in

4 MODEL VERIFICATION

For the first example we took a 60-mm-diameter cylinder of 0.43% carbon steel quenched from 870°C into water. This example was analyzed theoretically and experimentally by [13] and [14] and also theoretically by [20].

From the published data we estimated the value of the coefficient of heat transfer to be near 25 kW/m^{2}K. It should be mentioned that even with such a high value for the coefficient of convection heat transfer we could not obtain the cooling speed at the centre of the cylinder which was reported by [13]. Nevertheless, the calculated residual stresses were in good agreement with experimental values, as can be seen from Fig.1.

As a second example we considered cylinders of diameters 10 mm, 30 mm, 50 mm and 100 mm made from 0.44% carbon steel. The axial residual stress distribution for these cylinders was investigated experimentally by [2] and theoretically by [23]. All the cylinders were quenched into water at 20 °C from a temperature of 850 °C. For the coefficient of convective heat transfer we



Sl 1. *Zaostale napetosti v gašenem valju premera 60 mm*
Fig. 1. *Residual stress distribution in a 60 mm-diameter quenched cylinder*

5700 W/m^{2}K. Prav tako smo izvedli izračun s konvekcijskim koeficientom, ki je temperaturno odvisen in katerega odvisnost je iz podatkov [12].

took values for the constants between 3200 W/m^{2}K and 5700 W/m^{2}K. We also performed calculations with the temperature-dependent coefficient of convective heat transfer, which was calculated from the experimental data given by [12]

$$h = 1029 + 63\,\vartheta - 0{,}14\,\vartheta^2 + 0{,}7510^{-4}\,\vartheta^3 \quad \mathrm{W/m^2K} \tag{51}$$

Na slikah 2 do 5 so poleg izračunanih osnih napetosti podane tudi eksperimentalne vrednosti, ki so jih podali [2] in [23]. Kakor se vidi iz teh slik, se izračunane vrednosti za valje s premeri 30 mm, 50 mm in 100 mm dobro ujemajo z eksperimentalnimi vrednostmi. Za valj premera 10 mm so vrednosti zaostalih napetosti, ki jih podaja [2] negativne, tiste, ki jih podaja [23], pa so pozitivne, zato se nismo mogli odločiti, ali so izračunane vrednosti prave.

In figures 2 to 5 the calculated residual axial stresses are shown together with the experimental values given by [2] and [23]. As can be seen from these figures the calculated residual stresses for the cylinders of diameter 30 mm, 50 mm and 100 mm are in very good agreement with the experimental values. For the 10 mm-diameter cylinder the value of the residual stress given by [2] is negative and that given by [23] is positive, so we could not conclude that the calculated values are correct.

5 ANALIZA OBČUTLJIVOSTI

Z namenom, da določimo zanesljivost modela, smo izvedli analizo občutljivosti. Kot izhodni parameter modela smo vzeli osne zaostale napetosti na osi in robu valja. Za nadzor smo vzeli 36 materialnih parametrov. Če z a_k označimo parameter, potem je njegov relativni koeficient občutljivosti definiran z:

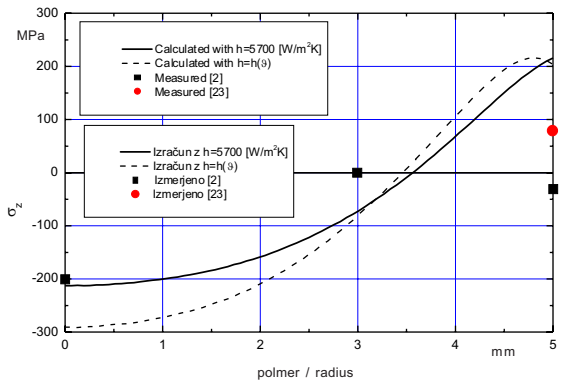
5 SENSITIVITY ANALYSIS

In order to estimate the accuracy of the model we performed a sensitivity analysis. As an output parameter from the model we took the axial residual stress on the axis of the cylinder and on its boundary. For the control parameters we took 36 material parameters. If we denote these parameters as a_k then the relative sensitivity coefficient is defined by:

$$s_k = \frac{a_k}{\sigma_z}\frac{\partial \sigma_z}{\partial a_k} \tag{52}$$

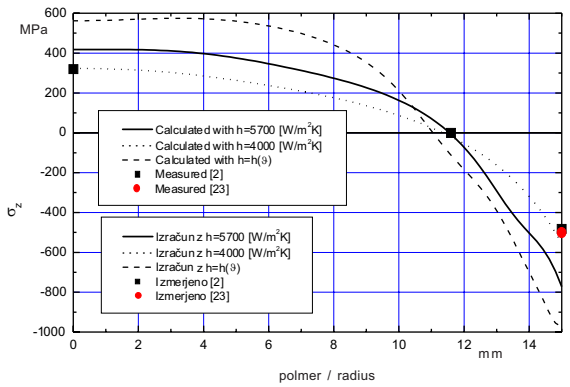
Izračun koeficientov občutljivosti smo izvedli za valje s premerom 10 mm, 30 mm in 50 mm. Parcialne odvode v (52) smo izračunali numerično. Podatki in rezultati izračuna so podani v preglednici 2.

We carried out the calculation of the sensitivity coefficients for cylinders of diameter 10 mm, 30 mm and 50 mm. The partial derivatives in (52) were performed by numerical differentiation The data and the results of the calculation are shown in Table 2.



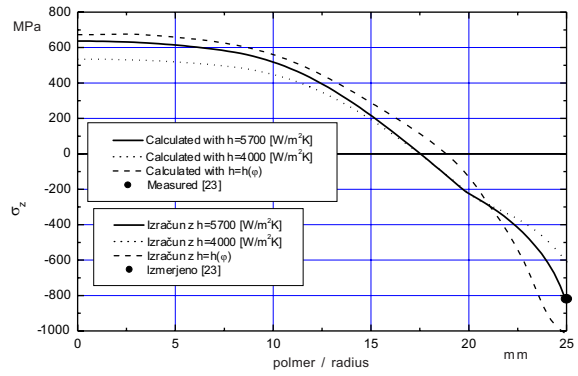
Sl. 2. *Osne zaostale napetosti v gašenem valju premera 10 mm*

Fig. 2. *Axial residual stress distribution in a quenched 10 mm diameter cylinder*



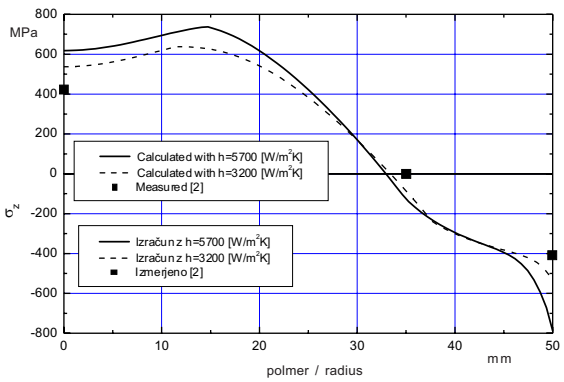
Sl. 3. *Osne zaostale napetosti v gašenem valju premera 30 mm*

Fig. 3. *Axial residual stress distribution in a quenched 30 mm diameter cylinder*



Sl. 4. *Osne zaostale napetosti v gašenem valju premera 50 mm*

Fig. 4. *Axial residual stress distribution in a quenched 50 mm diameter cylinder*



Sl. 5. *Osne zaostale napetosti v gašenem valju premera 100 mm*

Fig. 5. *Axial residual stress distribution in a quenched 100 mm diameter cylinder*

Iz preglednice 2 vidimo, da so v skoraj vseh primerih najvplivnejši parametri model temperaturni razteznostni koeficient austenita α_A, dilatacija austenita γ_A in martenzita γ_M, ekstremna točka na krivulji TTT za perlit (t_P,P_m) in bainit (t_B,B_m) in nazadnje temperaturi A_3 in B_s. Prav tako je model nekoliko občutljiv za konvekcijski koeficient h in masni delež ogljika C.

Iz povedanega sklepamo, da je model zelo občutljiv za kinetiko prehoda austenita v perlit in bainit. V primeru valja s premerom 10 mm, ko se skoraj celoten valj spremeni v martenzit, je model tudi zelo občutljiv za parametre kinetične enačbe (34). Po drugi strani pa je model razmeroma neobčutljiv za mejo plastičnega tečenja in druge mehanske in fizikalne lastnosti.

Na temelju koeficientov občutljivosti smo ocenili relativno napako izračunanih zaostalih napetosti po obrazcu:

From table 2 we can see that the most important parameters in the model are, in almost all cases: the thermal expansion of austenite α_A; the dilatation of austenite γ_A and martensite γ_M; the extreme points on the TTT curve for prearlite (t_P,P_m) and bainite (t_B,B_m);and finally, the temperatures A_3 and B_s. Also, the model is only moderately sensitive to the coefficient of convective heat transfer (h) and the weight percent of carbon.

From the above we can conclude that the model is very sensitive to the kinetics of phase change from austenite to pearlite and bainite. In the case of the 10-mm-diameter cylinder, where almost all the cylinder is transformed to martensite, the model is also very sensitive to parameters in the martensite kinetic equation (34). On the other hand, the model is relatively insensitive to yield stresses and other mechanical and physical data.

On the basis of sensitivity coefficients we can estimate the relative error of the residual stress with the formula:

$$\varepsilon_\sigma = \sqrt{\frac{1}{M}\sum_{i=1}^{M}\left(s_i\varepsilon_i\right)^2} \qquad (53),$$

Preglednica 2. *Podatki o materialu in izračunani koeficienti občutljivosti za valje premera 10, 30 in 50 mm*
Table 2. *Material data and calculated sensitivity coefficients for cylinders with diameter 10, 30 and 50 mm*

d				10 mm		30 mm		50 mm	
par.	enota unit	vrednost value	območje ± range ±	središče center	površina surface	središče center	površina surface	središče center	površina surface
c_P	MJ/m^{3}K	3,76	0,15	-0,379	0,133	0,980	0,053	-0,271	-0,110
c_A	MJ/m^{3}K	4,15	0,2	-0,844	-0,857	-0,607	-0,577	0,144	-0,455
λ_P	W/mK	66,20	1,74	-0,126	-0,030	-4,280	-2,127	-0,198	-0,833
λ_A	W/mK	15	0,573	-0,021	0,678	0,573	-0,424	-0,448	-0,348
λ_M	W/mK	25	1,74	-0,279	-0,644	0,011	-0,082	0,007	-0,003
l_{PA}	MJ/m^3	630	30	-0,065	-0,074	0,420	0,042	0,063	-0,242
l_{MA}	MJ/m^3	660	30	-0,257	-0,090	-0,013	-0,013	-0,002	-0,002
E_P	GPa	209	1,26	0,646	1,680	1,654	1,227	1,034	0,129
E_A	GPa	200	0,32	-0,188	0,313	-0,188	-0,063	-0,188	0
ν	-	0,30	0,01	0,171	0,894	0,711	0,501	0,402	0,033
α_A	10^{-4} K^{-1}	22	1	-3,971	-5,223	8,452	0,363	10,86	0,147
α_B	10^{-4} K^{-1}	13	1	-0,138	-0,099	-1,017	0,049	-0,052	-0,044
α_P	10^{-4} K^{-1}	14	1	-0,206	-0,218	-0,678	1,740	-4,572	0,078
α_M	10^{-4} K^{-1}	12	1	0,714	1,188	-0,132	-0,634	0	0,002
γ_M	10^{-3}	8,50	0,22	4,165	4,857	0,042	0,742	-0,008	0
γ_A	10^{-3}	10,7	0,7	5,397	6,385	-6,629	0,214	-7,453	-0,113
K_M	10^{-5} MPa^{-1}	4,18	0,1	-0,021	0,004	-0,217	-0,059	-0,385	0,008
K_B	10^{-5} MPa^{-1}	5,08	0,1	-1,483	-0,320	-0,218	-0,742	0,005	0,005
σ_Y^P	MPa	434	34	-0,006	-0,049	0,005	0	0,794	0,128
σ_Y^B	MPa	491	34	-0,003	-0,023	0	0	0,143	0,459
σ_Y^A	MPa	123	2	-0,062	-0,597	0,068	0,012	0,062	-0,012
σ_Y^M	MPa	445	30	0	0	0	0	0,013	0,323
ϑ_s	°C	850	20	0,315	0,196	-1,441	-2,809	1,687	-2,265
ϑ_f	°C	20	5	-0,228	-0,145	-0,112	-0,246	-0,093	-0,153
h	W/m^{2}K	5700	700	2,017	1,228	0,812	2,018	0,571	1,523
k_M	-	0,011	0,0005	3,793	3,181	0,110	0,539	0,002	0,086
B_m	°C	460	20	3,190	2,082	-0,435	4,791	-0,520	2,272
P_m	°C	560	20	4,819	3,693	5,547	2,918	2,111	4,460
t_B	s	1,3	0,1	1,080	0,849	0,260	0,922	-0,030	0,524
t_P	s	1	0,1	1,330	1,126	-0,816	0,110	0,054	0,779
A_3	°C	910	10	-5,260	-4,186	4,150	-1,338	4,359	-3,749
B_s	°C	830	25	-3,552	-2,590	0,445	-3,801	-0,601	-1,829
M_s	°C	539	25	-0,388	-1,150	0,296	1,156	0,024	0,559
C	-	0,44	0,02	1,340	1,547	1,816	0,537	2,080	1,155
Mn	-	0,66	0,1	0,391	0,349	-0,145	0,237	-0,052	0,177
Si	-	0,22	0,07	-0,057	-0,046	0,045	-0,014	0,047	-0,041

pri čemer je ε_i relativna napaka *i* tega parametra. Z uporabo podatkov iz preglednice 2 smo izračunali oceno relativne napake izračunanih zaostalih napetosti. Rezultati so podani v preglednici 3.

where ε_i is the relative error of *i*th parameter. By using data from Table 2 the estimated relative error in the residual stresses are calculated. The results are shown in Table 3.

Preglednica 3. *Ocenjene relativne napake osnih napetosti*
Table 3. *Estimated relative errors of the axial residual stresses*

d [*mm*]	Središče Center	Površina Surface
10	0,11	0,11
30	0,11	0,07
50	0,13	0,05

6 SKLEP

Izdelan je bil matematični model toplotne obdelave in zbrani vsi potrebni podatki. Model smo uspešno preskusili na dveh primerih izračuna zaostalih napetosti, za katere so znani eksperimentalni rezultati. Nadalje smo izvedli analizo občutljivosti modela, s katero smo dobili kolikostno oceno vplivnosti posameznih podatkov v materialu. Prav tako je bila ocenjena relativna napaka v izračunu zaostalih napetosti.

Na podlagi tega so glavne ugotovitve:

1. model toplotne obdelave je izredno občutljiv za podatke, ki so vključeni v kinetičnih enačbah;
2. model je prav tako pomembno občutljiv za temperaturni razteznostni koeficient austenita in dilatacijski koeficient prehoda med austenitom in martenzitom;
3. relativna napaka pri izračunu zaostalih napetosti je ocenjena na 13%.

6 CONCLUSIONS

We have developed a mathematical model for heat treatment and collected the necessary data needed for practical calculations. We successfully tested the model in two examples for which the experimental data were available. We then performed a sensitivity analysis of the model which resulted in a quantitative determination of the relative importance of the various material data. The relative error in the calculated residual stresses was also estimated.

The main conclusions are as follows:

1. the model of heat treatment is very sensitive to the data which are used in the kinetic equations;
2. the model is also very sensitive to the austenite thermal expansion coefficient and the dilatation of austenite and martensite;
3. the calculated relative error for the residual stresses, using data published in the literature, are within 13%.

7 LITERATURA
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