SIMULATION OF QUENCHING PROCESS USING THE FINITE ELEMENT METHOD

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Abstract. *This contribution is concerned with modeling and simulation of quenching employing the finite element method. An anisothermal constitutive model formulated within the framework of continuum mechanics and the thermodynamics of irreversible processes is considered adopting two phases: austenite and martensite. A numerical procedure is developed based on operator split technique associated with an iterative numerical scheme in order to deal with nonlinearities in the formulation. With this assumption, coupled governing equations are solved involving four uncoupled problems: thermal, phase transformation, thermoelastic and elastoplastic behaviors. Classical finite element method is employed for spatial discretization of thermal and thermoelastic uncoupled problems. Progressive induction hardening of steel cylinders is concerned as an application of the general procedure. A comparison between numerical and experimental measures is performed showing good agreements between them.*

Keywords*. Quenching, Phase transformation, Finite element, Modeling.*

1. Introduction

Quenching is a heat treatment usually employed in industrial processes. It provides a mean to control mechanical properties of steels. The process consists of raising the steel temperature above a certain critical value holding it at that temperature for a fixed time, and then rapidly cooling it in a suitable medium to room temperature. The resulting microstructures formed from quenching (ferrite, pearlite, bainite and martensite) depend on cooling rate and steel characteristics. Considerable residual stresses may be formed during quenching process and therefore, its prediction is an important task (Inoue and Raniecki, 1978; Sjöström, 1985; Denis et al., 1985; Denis et al., 1992; Denis et al., 1999; Fernandes et al., 1985; Woodard et al., 1999; Sen et al., 2000; Çetinel et al., 2000; Gür and Tekkaya, 2001). Nevertheless, the proposed models are not generic and are usually applicable to simple geometries as cylinders. Several authors addressed Finite Element Method (FEM) in order to analyze quenching process. Sen et al. (2000) considers steel cylinders without phase transformations. Other authors considered simple geometries with phase transformations (Çetinel et al., 2000; Gür and Tekkaya, 2001; Chen et al., 1997; Gür and Tekkaya, 1996). Gür et al. (1996) studied the effect of the refrigerant medium in cylinders with an eccentric hole.

Phenomenological aspects of quenching involve couplings among different physical processes and its description is unusually complex. Basically, three couplings are essential: thermal phenomena, phase transformation and mechanical aspects. Complex aspects as the heat generated during phase transformation are treated by some authors considering the latent heat associated with phase transformation (Denis et al., 1999; Inoue and Wang, 1985; Denis et al., 1987; Sjöström, 1994). Meanwhile, other coupling terms in the energy equation related to other phenomena as plastic strain or hardening are not treated in literature and their analysis is an important topic to be investigated. Pacheco et al. (1997; 2001a; 2001b) and Silva et al. (2002) propose a constitutive model to describe the thermo-mechanical behavior related to the quenching process. This anisothermal model is formulated within the framework of continuum mechanics and the thermodynamics of irreversible processes considering two phases: austenite and martensite. The proposed approach is general and allows a direct extension to more complex situations. The model includes thermomechanical couplings in the energy equation associated with phase transformation, plasticity and hardening, allowing the investigation of the effects promoted by these coupling (Silva et al., 2002).

The present contribution uses the cited constitutive model associated with FEM in order to simulated quenching process. As an application of the general formulation plane elements are adopted which allows the description of axisymmetrical problems. The extension to other element types is a direct task. Comparisons between numerical and experimental measures of steel cylinders are carried out in order to validate results.

2. Constitutive Model

The thermodynamic state of a solid is completely defined by the knowledge of state variables. Constitutive equations may be formulated within the framework of continuum mechanics and the thermodynamics of irreversible processes, by considering thermodynamic forces, defined from the Helmholtz free energy, ψ, and thermodynamic fluxes, defined from the pseudo-potential of dissipation, ϕ (Pacheco et al., 2001a; Pacheco et al., 2001b; Silva et al., 2002).

A Helmholtz free energy is proposed as a function of observable variables, total deformation, ε_{ij}, and temperature, T; also, internal variables are considered: plastic deformation, ε_{ij}^{p}, volumetric fraction of martensitic phase, β, and another set of variables associated with phase transformation, hardening and other effects as damage. Here, this set considers a variable related to kinematic hardening, α_{ij}. Therefore, the following free energy is considered, presented in indicial notation where summation convention is evoked (Eringen, 1967):

$$\rho\,\psi(\varepsilon_{ij},\varepsilon_{ij}^{p},\alpha_{ij},\beta,T)=W(\varepsilon_{ij},\varepsilon_{ij}^{p},\alpha_{ij},\beta,T) \tag{1}$$

where $\varepsilon_{ij}^{e}=\varepsilon_{ij}-\varepsilon_{ij}^{p}-\alpha_T(T-T_0)\delta_{ij}-\gamma\beta\delta_{ij}-(3/2)\kappa\sigma_{ij}^{d}\beta(2-\beta)$ is the elastic deformation, α_T is the coefficient of linear thermal expansion and γ and κ are material parameters related to expansion and plastic deformation induced by martensitic transformation (Sjöström, 1985; Denis et al., 1985). The deviatoric stress component is defined by $\sigma_{ij}^{d}=\sigma_{ij}-\delta_{ij}(\sigma_{kk}/3)$.

Thermodynamics forces (σ_{ij}, P_{ij}, X_{ij}, B^{β}, s), associated with state variables $(\varepsilon_{ij},\varepsilon_{ij}^{p},\alpha_{ij},\beta,T)$, are defined as follows:

$$\begin{aligned}\sigma_{ij}&=\frac{\partial W}{\partial\varepsilon_{ij}}=\Phi_{ijpq}E_{pqkl}\left[\varepsilon_{kl}-\varepsilon_{kl}^{p}-\left(\alpha_T(T-T_0)+\gamma\beta\right)\delta_{kl}\right]+\\&+\Phi_{ijpq}E_{pqkk}\left[\frac{1}{2}\kappa\beta(2-\beta)\right]\left\{\frac{\Phi_{aaef}E_{efrs}\left[\varepsilon_{rs}-\varepsilon_{rs}^{p}-\left(\alpha_T(T-T_0)+\gamma\beta\right)\delta_{rs}\right]}{1-\Phi_{bbcd}E_{cdgg}\left[\frac{1}{2}\kappa\beta(2-\beta)\right]}\right\}\end{aligned} \tag{2}$$

$$P_{ij}=-\frac{\partial W}{\partial\varepsilon_{ij}^{p}}=\sigma_{ij}\quad;\quad X_{ij}=\frac{\partial W}{\partial\alpha_{ij}}=H_{ijkl}\alpha_{kl}\quad;\quad s=-\frac{1}{\rho}\frac{\partial W}{\partial T} \tag{3}$$

$$B^{\beta}=-\frac{\partial W}{\partial\beta}=-\left(\frac{\partial W_e}{\partial\beta}+Z\right)=E_{pqkl}\left(\varepsilon_{ij}-\varepsilon_{ij}^{p}\right)\left\{A_{ijpqkl}+\frac{E_{efrs}\delta_{kl}}{\Xi}\left[B_{ijpqefrs}+M_{ijpqefrs}+\frac{N_{ijpqefrs}}{\Xi}\right]\right\}-Z \tag{4}$$

where $\Phi_{ijpq}=C_{ijpq}^{-1}$ and $C_{ijpq}=\delta_{pi}\delta_{qj}+\frac{3}{2}E_{ijpq}\kappa\beta(2-\beta)$.

$I_{\beta}(\beta)$ is the indicator function related to the convex set $C_{\beta}=\{\beta\mid 0\le\beta\le 1\}$ (Rockafellar, 1970). Moreover,

$$\Xi=1-\Phi_{zzhn}E_{hnxx}\left[\frac{1}{2}\kappa\beta(2-\beta)\right]\quad;\quad A_{ijpqkl}=\frac{\partial\Phi_{ijpq}}{\partial\beta}\left\{\left(\alpha_T(T-T_0)+\gamma\beta\right)\delta_{kl}-\frac{1}{2}\left(\varepsilon_{kl}-\varepsilon_{kl}^{p}\right)\right\}+\Phi_{ijpq}\gamma\delta_{kl} \tag{5}$$

$$B_{ijpqefrs}=\left[\frac{1}{2}\kappa\beta(2-\beta)\right]\left(\frac{\partial\Phi_{ijpq}}{\partial\beta}\Phi_{aaef}+\Phi_{ijpq}\frac{\partial\Phi_{aaef}}{\partial\beta}\right)\left\{\left(\alpha_T(T-T_0)+\gamma\beta\right)\delta_{rs}-\frac{1}{2}\left(\varepsilon_{rs}-\varepsilon_{rs}^{p}\right)\right\} \tag{6}$$

$$M_{ijpqefrs}=\Phi_{ijpq}\Phi_{aaef}\left\{\kappa(1-\beta)\left(\left(\alpha_T(T-T_0)+\gamma\beta\right)\delta_{rs}-\frac{1}{2}\left(\varepsilon_{rs}-\varepsilon_{rs}^{p}\right)\right)+\gamma\left[\frac{1}{2}\kappa\beta(2-\beta)\right]\delta_{rs}\right\} \tag{7}$$

$$N_{ijpqefrs}=\Phi_{ijpq}\left[\frac{1}{2}\kappa\beta(2-\beta)\right]\Phi_{aaef}\left\{E_{cdgg}\left(\frac{\partial\Phi_{bbcd}}{\partial\beta}\left[\frac{1}{2}\kappa\beta(2-\beta)\right]+\Phi_{bbcd}\kappa(1-\beta)\right)\right\}\left\{\left(\alpha_T(T-T_0)+\gamma\beta\right)\delta_{rs}-\frac{1}{2}\left(\varepsilon_{rs}-\varepsilon_{rs}^{p}\right)\right\} \tag{8}$$

$Z \in \partial_\beta I_\beta(\beta)$ is the sub-differential of the indicator function I_β (Rockafellar, 1970).

Austenite-martensite phase transformation is described with the aid of the following condition:

$$\varsigma_{A\to M}\left(\dot{T},T\right)=\Gamma\left(\left|\dot{T}\right|-rMs\right)\cdot\Gamma\left(M_s-T\right)\cdot\Gamma\left(T-M_f\right) \tag{9}$$

where rM_s is the critical cooling rate for the martensite formation, defined from the continuous cooling transformation (CCT) diagram; $\dot{T}$ is the cooling rate. Also, $\Gamma(x)$ is the Heaviside function (Wang et al., 1997). Therefore, using the equation proposed by Koistinen and Marburger (Koistinen and Marburger, 1959) to express the kinetics of phase transformation, it is possible to write:

$$\beta=\beta\left(T,\dot{T}\right)=\varsigma_{A\to M}\,\beta^m=\varsigma_{A\to M}\,\{1-\exp[-k(M_s-T)]\} \tag{10}$$

here, k is a material constant. M_s is the temperature where martensite starts to form in the stress-free state and M_f is the temperature where martensite finishes its formation in the stress-free state.

In order to describe dissipative processes, it is necessary to introduce a potential of dissipation $\phi(\dot{\varepsilon}_{ij}^p,\dot{\alpha}_{ij},\dot{\beta},q_i)$, which can be split into two parts: $\phi(\dot{\varepsilon}_{ij}^p,\dot{\alpha}_{ij},\dot{\beta},q_i)=\phi_1(\dot{\varepsilon}_{ij}^p,\dot{\alpha}_{ij},\dot{\beta})+\phi_2(q_i)$. Also, this potential can be written through its dual $\phi^*(P_{ij},X_{ij},B^\beta,g_i)=\phi_1^*(P_{ij},X_{ij},B^\beta)+\phi_2^*(g_i)$. With this assumption, thermodynamic fluxes may be written as

$$\dot{\varepsilon}_{ij}^p\in\partial_{P_{ij}}I_f^*(P_{ij},X_{ij})=\lambda\,\mathrm{sign}\left(\sigma_{ij}-H_{ijkl}\alpha_{kl}\right)\quad;\quad\dot{\alpha}_{ij}\in-\partial_{X_{ij}}I_f^*(\sigma_{ij},X_{ij})=\dot{\varepsilon}_{ij}^p\quad;\quad\dot{\beta}=\frac{\partial\phi^*}{\partial B^\beta}=\varsigma_{A\to M}\,\dot{\beta}^m \tag{11}$$

$$q_i=-\frac{\partial\phi^*}{\partial g_i}=-\Lambda T\,g_i=-\Lambda\frac{\partial T}{\partial x_i} \tag{12}$$

where sign(x) = x / $|x|$ and λ is the plastic multiplier from the classical theory of plasticity (Lemaitre and Chaboche, 1990); q_i is the heat flux vector, $g_i = (1/T)\,\partial T/\partial x_i$ and Λ is the coefficient of thermal conductivity which is function of temperature; $I_f^*(P_{ij},X_{ij})$ is the indicator function associated with elastic domain, related to the *von Mises* criterion (Lemaitre and Chaboche, 1990),

$$f(P_{ij},X_{ij})=\left[\frac{3}{2}(P_{ij}^d-X_{ij}^d)(P_{ij}^d-X_{ij}^d)\right]^{1/2}-\sigma_Y\le 0 \tag{13}$$

σ_Y is the material yield stress, $X_{ij}^d = X_{ij} - \delta_{ij}(X_{kk}/3)$ and $P_{ij}^d=\sigma_{ij}^d$.

Assuming that the specific heat is $c=-(T/\rho)\,\partial^2 W/\partial T^2$ and the set of constitutive equations (2-4, 11-12), the energy equation can be written as (Pacheco, 1994):

$$\frac{\partial}{\partial x_i}\left(\Lambda\frac{\partial T}{\partial x_i}\right)-\rho c\dot{T}=-a_I-a_T \tag{14}$$

The term a_I is denoted as internal coupling and is always positive. The term a_T denotes the thermal coupling and can be either positive or negative. In this article both terms are neglected and thermal problem is solved as a rigid body.

3. Finite Element Formulation

In order to deal with the nonlinearities of the formulation, an iterative numerical procedure is proposed based on the operator split technique (Ortiz at al., 1983). With this assumption, coupled governing equations are solved from four uncoupled problems: thermal, phase transformation, thermo-elastic and elastoplastic. In this article, finite element method is employed to perform spatial discretization of governing equations. Therefore, the following moduli are considered:

Thermal Problem - Comprises a radial conduction problem with surface convection. Material properties depend on temperature and, therefore, the problem is governed by nonlinear parabolic equations. Classical finite element method is employed for spatial discretization while *Crank-Nicolson* method is used for time discretization (Lewis at al., 1996; Gartling and Hogan, 1994; Segerlind, 1984).

Phase Transformation Problem - Volumetric fraction of martensitic phase is determined in this problem. Evolution equations are integrated from a simple implicit Euler method (Pacheco et al., 2001a; Pacheco et al., 2001b; Ames, 1992; Nakamura, 1993).

Thermo-elastic Problem - Stress and displacement fields are evaluated from temperature distribution. Classical finite element method is employed for spatial discretization (Segerlind, 1984).

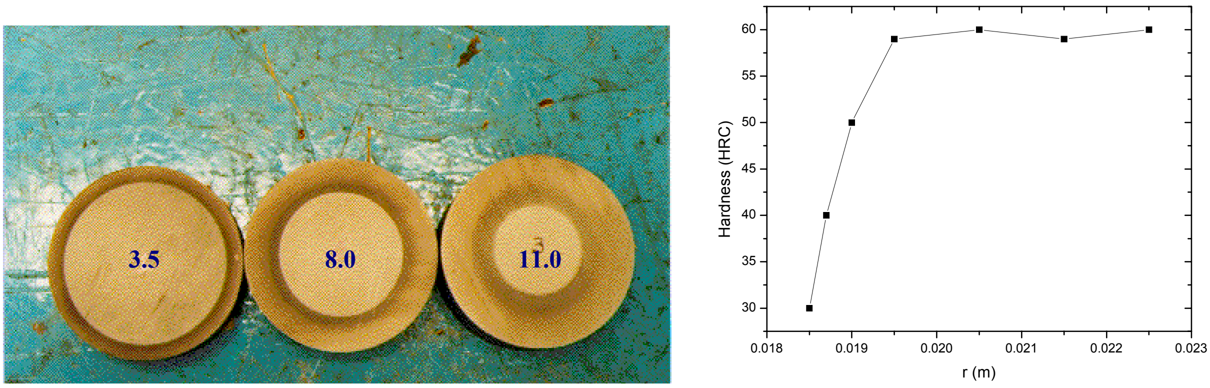
Elastoplastic Problem - Stress and strain fields are determined considering the plastic strain evolution in the process. Numerical solution is based on the classical return mapping algorithm (Pacheco et al., 2001a; Pacheco et al., 2001b; Simo and Hughes, 1998).

As an application of the general procedure technique, plane axisymmetric FEM is considered. Triangular elements with linear shape functions are adopted for all finite element moduli (Segerlind, 1984).

4. Numerical Simulation

As an application of the general proposed model, numerical investigations associated with the progressive induction (PI) hardening of long steel cylindrical bar are carried out. PI hardening is a heat treatment process that is done moving a workpiece at a constant speed through a coil and a cooling ring. Applying an alternating current to the coil, a magnetic field is generated which induces eddy currents that promote the heating of a thin surface layer where austenite is formed. After that, this layer is cooled transforming austenitic phase into martensite, pearlite, bainite and proeutectoid ferrite/cementite depending on, among other things, the cooling rate. A hard surface layer with high compressive residual stresses, combined with a tough core with tensile residual stresses, is often obtained.

This article considers PI hardening simulations in a cylindrical bar with radius R and a thickness of induced layer, e_{PI}. Experimental measures are used as reference values considering a steel cylinder SAE 4140H, 45 mm diameter and 180 mm length, subjected to different induced layers thickness e_{PI} (3.5mm, 8.0mm and 11.0mm), where the hardness is greater than HRC 40. The specimen induced layer is heated to 1120K (850°C) for 5s and then, the surface is sprayed by a liquid medium at 294K (21°C) for 10s. After that, the specimen is subjected to air-cooling until a time instant of 60s is reached (Camarão, 1998; Melander, 1985a; Melander, 1985b). Figure (1*a*) shows cross-sections of quenched bars with different induced layers thickness subjected to a Nital etch 2%. Figure (1*b*) presents its Rockwell C hardness measures for an induced layer thickness of 3.5 mm. Moreover, stress values on the surface layer are estimated using the X-ray diffraction peak technique (Camarão, 1998).



(a) (b)

Figure 1. (*a*) Cross-sections of quenched bars with different induced layers thickness submitted to a Nital etch 2%. (*b*) Rockwell C hardness measures for an induced layer thickness of 3.5 mm (Pacheco et al., 2001a; Pacheco et al., 2001b; Camarão, 1998; Camarão et al., 2000).

Material parameters for numerical simulation are presented in Tab. (1). Other parameters depend on temperature and are interpolated from experimental data (Pacheco et al., 2001a; Pacheco et al., 2001b; Melander, 1985a; Melander, 1985b; Hildenwall, 1979). Convection heat transfer coefficient for cooling fluid (Ucon E 2.8%) and air are also interpolated from experimental data (Pacheco et al., 2001a; Pacheco et al., 2001b; Melander, 1985a; Melander, 1985b; Camarão, 1998; Hildenwall, 1979).

Table 1. Material parameters (SAE 4140H).

$k = 1.100 \times 10^{-2}\ K^{-1}$	$\kappa = 5.200 \times 10^{-11}\ Pa^{-1}$	$M_s = 748$ K
$\gamma = 1.110 \times 10^{-2}$	$\rho = 7.800 \times 10^{3}\ kg/m^3$	$M_f = 573$ K

FEM analysis is performed exploiting the axisymmetrical geometry of the cylinder. A single strip of the cylinder is assumed to model the quenching process (Gür and Tekkaya, 1996). This assumption is employed since the passage of the moving workpiece through the heating and cooling rings induces their effects in this single strip while adjacent material, above and below this strip, is at lower temperatures. The material at lower temperatures prevents the axial strain and, as a consequence, plane strain condition may be adopted. Moreover, radial heat flux is assumed.

Figure (2) shows a mesh with 488 nodes and 842 elements employed in numerical simulations after a convergence analysis. The segment *OM* is at the cylinder center axis while *LK* is at the cylinder surface. Null displacements conditions are imposed in *OK* and *ML*. Moreover, thermal boundary conditions impose convection condition in *KL* while other faces have adiabatic conditions.

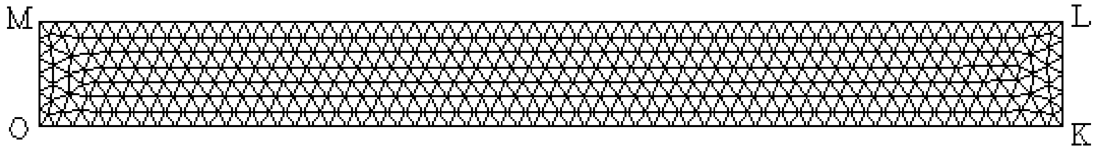


Figure 2. Mesh employed for finite element analysis.

Figure (3) shows the distribution of volumetric fraction of martensite, β, for the final time instant considering different thickness of induced layer, e_{PI}. Figure (4) establishes a comparison between experimental and numerical results for e_{PI} = 3.5 mm showing that they are in close agreement.

The forthcoming analysis considers residual stresses in the final time instant for different thickness of induced layer, e_{PI} (Figs. 5-6). Component σ_r presents lower magnitudes than other components (σ_θ and σ_z). Components σ_θ and σ_z are always compressive in cylinder surface. As the thickness of induced layer, e_{PI}, increases, compressive components σ_θ present lower magnitudes (Fig. 5) while compressive components σ_z present higher magnitudes (Fig. 6).

A different way to observe previous results is analyzing the radial distribution of residual stress components (Fig. 7). An important characteristic to be pointed out is the sign inversions of the residual stress values, which defines different regions of the specimen. In general, induced layers of 3.5mm and 8.0mm have compressive stress in either the surface and the core of the cylinder. On the other hand, when e_{PI} = 11 mm, the surface has compressive stresses but the core present tensile stresses. This result is similar to the behavior of the through hardening (Pacheco et al., 2001a; Pacheco et al., 2001b). As the induced layer is reduced, values of σ_z become less negative at the surface tending to become positive when thin layers are assumed (Pacheco et al., 2001b). This condition must be avoided, since tensile stress field on the surface can promote the growth of surface defects. All these considerations show that the thickness of the induced layer is an important parameter on the residual stress distribution.

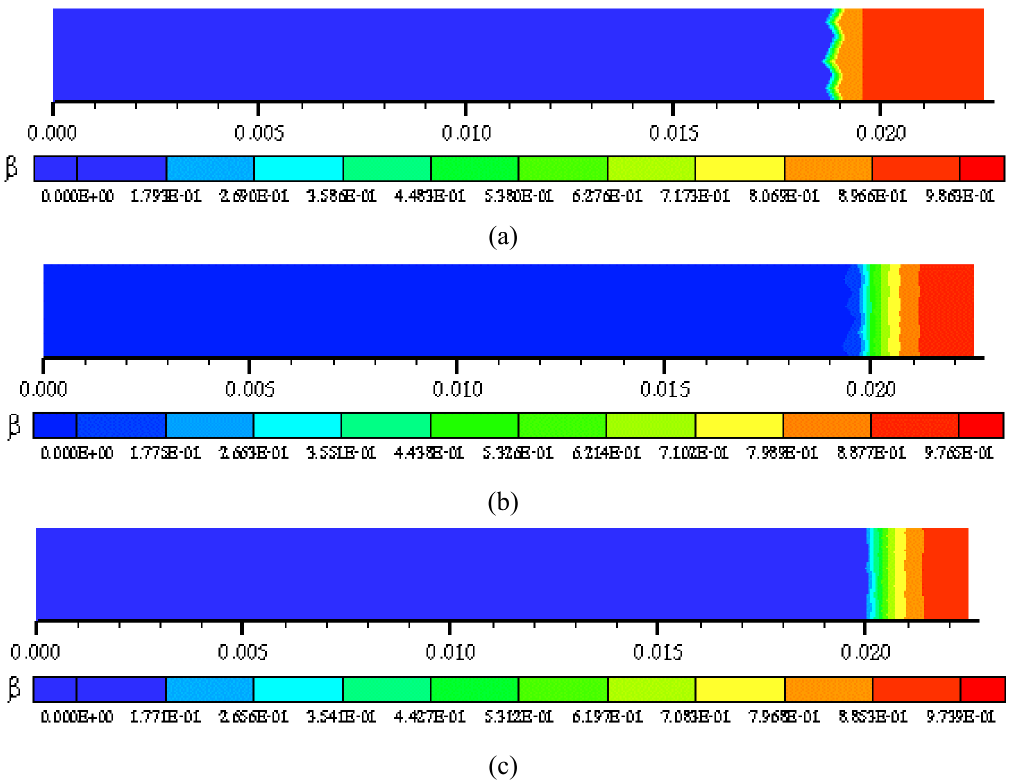


Figure 3. Volumetric fractions of martensite: (a) e_{PI} =3.5 mm; (b) e_{PI} =8.0 mm; (c) e_{PI} =11.0 mm.

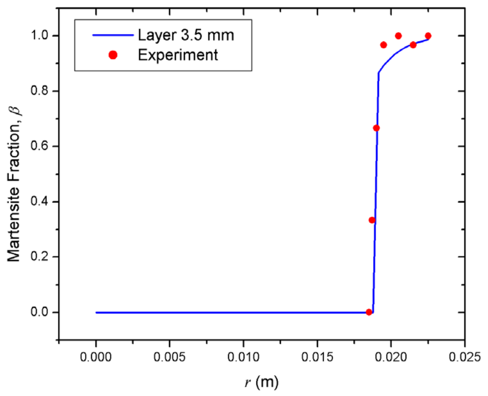


Figure 4. Comparison between numerical and experimental results: Volumetric fraction of martensite for e_{PI} = 3.5 mm (Pacheco et al., 2001a; Pacheco et al., 2001b; Camarão, 1998).

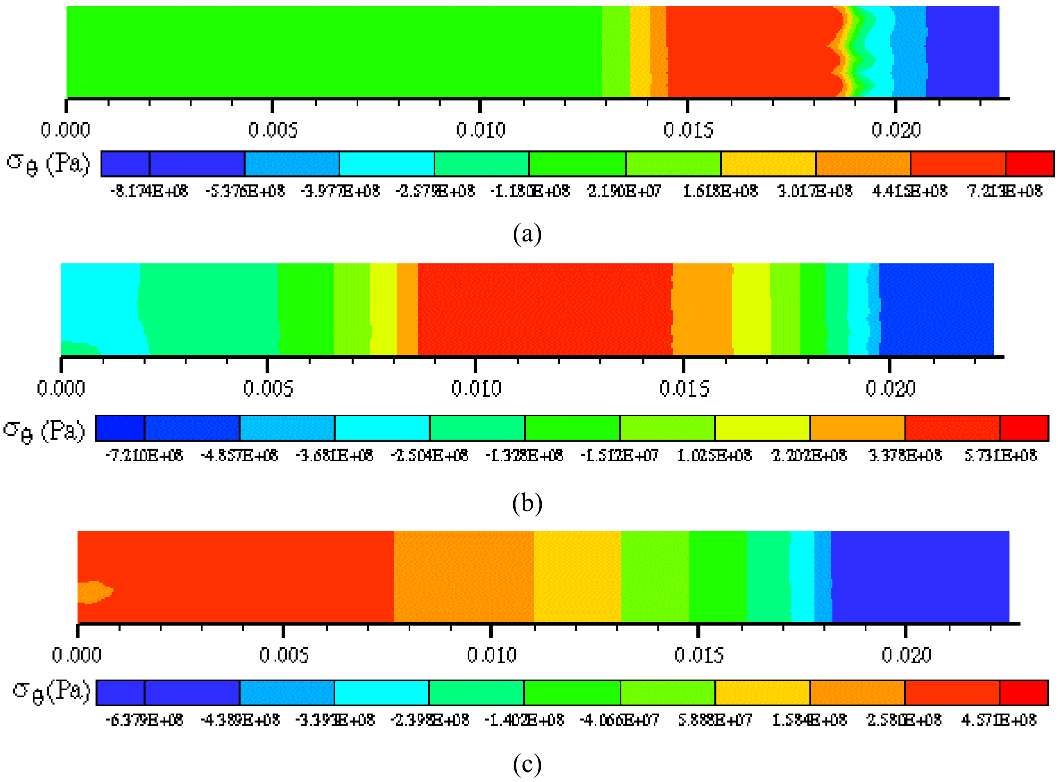
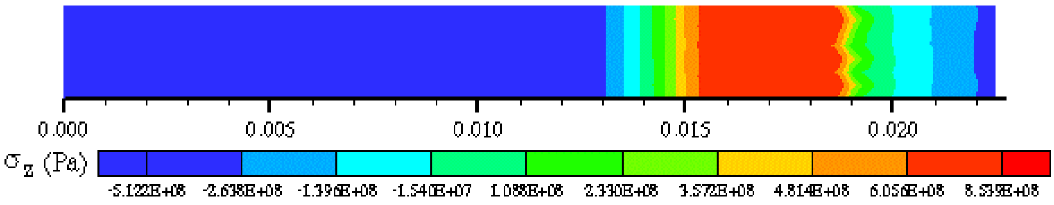
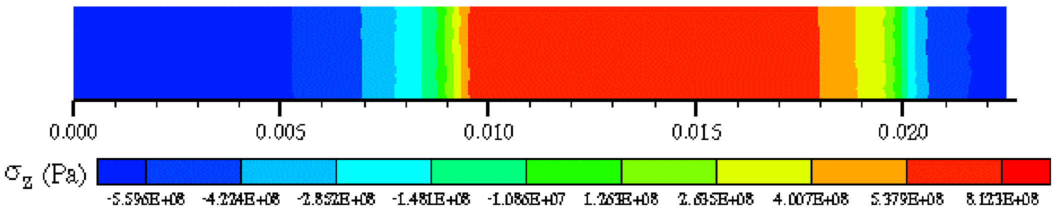


Figure 5. Residual stress σ_θ distribution for different e_{PI}: (a) 3.5 mm; (b) 8.0 mm; (c) 11.0 mm.



(a)



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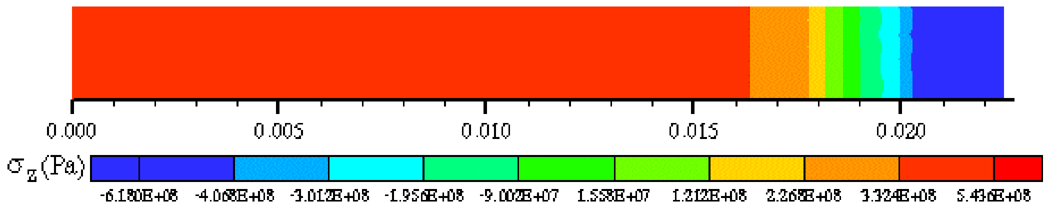
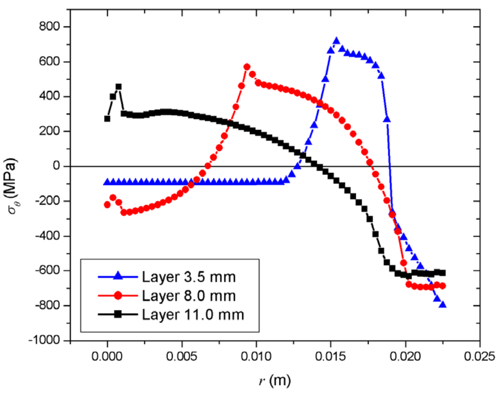
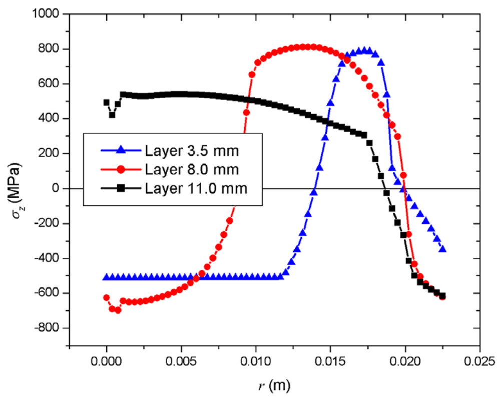


(c)

Figure 6. Residual stress σ_z distribution for different e_{PI}: (a) 3.5 mm; (b) 8.0 mm; (c) 11.0 mm.



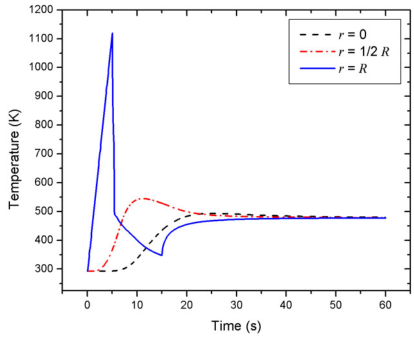
(a)



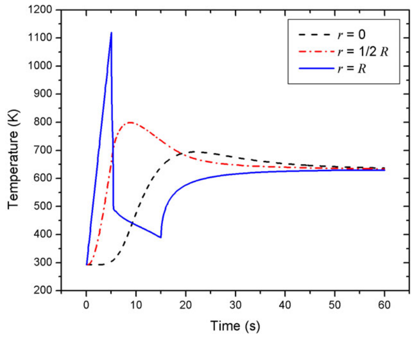
(b)

Figure 7. Residual stress distribution over the radius for the final time instant.(a) σ_θ; (b) σ_z.

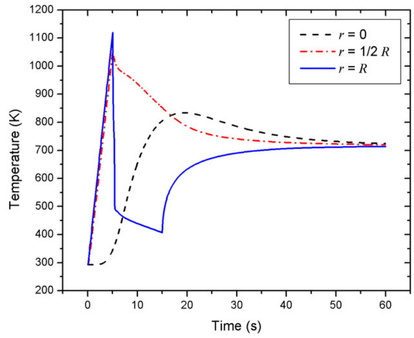
Temperature distribution tends to become homogeneous for any thickness of induced layer. Nevertheless, the time history is quite different. Figure (8) presents the effect of induced layer thickness in temperature distribution showing temperature time history for different radius positions: core (r = 0), midpoint (r = ½ R) and surface (r = R). Moreover, different values of induced layer thickness are considered. The surface temperature evolution allows one to identify two distinct cooling stages: in the liquid medium (5 < t ≤ 15 s) and in the air (t > 15 s).



(a)



(b)



(c)

Figure 8. Time history of temperature for different radius positions and e_{PI}: (a) 3,5 mm; (b) 8,0 mm; (c) 11,0 mm.

Table (2) establishes a comparison between numerical and experimental measures. For the induced layer thickness of 3.5 mm an error less than 2% is observed for both the circumferential stress, σ_θ, and longitudinal stress, σ_z. By increasing the induced layer thickness, an error less than 2% is still observed for the circumferential stress, σ_θ. The longitudinal stress, σ_z, on the other hand, presents a discrepancy (15% for induced layer thickness of 8 mm and 40% for induced layer thickness of 11 mm). These discrepancies could be assigned to plane strain state adopted in order to simulate quenching process. This assumption try to represent the restriction associated with adjacent regions of the heated region, which are at lower temperatures. By increasing induced layer thickness, temperature distributions tend to be essentially non-homogeneous promoting different strain distributions.

Table 2. Comparison between numerical and experimental measures.

e_{PI} (mm)	σ_θ (MPa)		σ_z (MPa)	
	Experimental	Numerical	Experimental	Numerical
3,5	–830	–817.4	–505	–512.2
8,0	–752	–721.0	–486	–559.6
11,0	–636	–637.9	–440	–618.0

5. Conclusions

The present contribution is concerned with modeling and simulation of quenching process, considering finite element method associated with an anisothermal constitutive model with two phases (austenite and martensite). A numerical procedure is developed based on operator split technique associated with an iterative numerical scheme in order to deal with nonlinearities in the formulation. With this assumption, coupled governing equations are solved involving four uncoupled problems: thermal, phase transformation, thermoelastic and elastoplastic behaviors. Classical finite element method is employed for spatial discretization in uncoupled problems. Progressive induction hardening of steel cylindrical bodies is considered as an application of the proposed general formulation. Numerical and experimental results are in agreement. The authors agree that the proposed model can be a useful tool to predict the thermomechanical behavior of quenched mechanical components. This is important for choosing essential parameters as the cooling medium and the induced layer thickness. It should be pointed out that the proposed approach is general, allowing a direct extension to more complex situations. The analysis of three-dimensional media and the inclusion of other phases can be easily achieved.

6. Acknowledgements

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