QUENCHING MODELING AND SIMULATION IN STEEL CYLINDERS

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Abstract. *Quenching is a commonly used heat treatment process employed to control the mechanical properties of steels. In brief, quenching consists of raising the steel temperature above a certain critical value, called austenitizing temperature, 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 (pearlite, ferrite, bainite and martensite) depend on cooling rate and on steel characteristics. This article deals with the themomechanical analysis of steel cylinders quenching. A multi-phase constitutive model is employed for its modeling and simulation. Experimental analysis related to temperature evolution during the process and its resulting microstructure is developed and is used as a reference for the modeling effort. The energy equation thermomechanical coupling terms are explored, considering two different models. The first one is an uncoupled model where thermomechanical couplings are neglected, corresponding to the rigid body energy equation. The second model considers the latent heat associated with phase transformation in order to represent thermomechanical coupling. The through hardening of a cylindrical body is considered as an application of the proposed general formulation. Numerical simulations present a good agreement with experimental data, indicating some situations where it is important to consider the thermomechanical coupling in the description of quenching process.*

Keywords. *Quenching, Phase Transformation, Thermomechanical Coupling, Modeling, Numerical Simulation, Experimental.*

1. INTRODUCTION

Quenching is a heat treatment usually employed in industrial processes. It provides a mean to control mechanical properties of steels as toughness and hardness. 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, cementite, pearlite, upper bainite, lower bainite and martensite) depend on cooling rate and on chemical composition of the steel. The volume expansion associated with the formation of martensite combined with large temperature gradients and non-uniform cooling can promote high residual stresses. As these internal stresses can produce warping and even cracking of a steel body, the prediction of such stresses is an important task.

Phenomenological aspects of quenching involve couplings among different physical processes and its description is unusually complex. Basically, three couplings are essential: thermal, phase transformation and mechanical phenomena. The description of each one of these phenomena has been addressed by several authors by considering these aspects separately. Sen *et al.* (2000) considers steel cylinders without phase transformations. There are also references focuses on the modeling of the phase transformation phenomenon (Hömberg, 1996; Chen *et al.*, 1997, Çetinel *et al.*, 2000; Reti *et al.*, 2001). Several authors have proposed coupled models that are not generic and are usually applicable to simple geometries as cylinders (Inoue & Wang, 1985; Melander, 1985; Sjöström, 1985; Denis *et al.*, 1985, 1987, 1999; Denis, 1996; Fernandes *et al.*, 1985; Woodard, *et al.*, 1999). Moreover, there are some complex aspects that are usually neglected in the analysis of quenching process. As an example, one could mention the heat generated during phase transformation. This phenomenon is usually treated by means of the latent heat associated with phase transformation (Inoue & Wang, 1985; Denis *et al.*, 1987, 1999; Sjöstrom, 1994; Woodward *et al.*, 1999). 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. Silva *et al.* (2004) analyze the thermomechanical coupling during quenching considering austenite-martensite phase transformations. Silva *et al.* (2005) employ the finite element method to the quenching analysis.

This article deals with the themomechanical analysis of steel cylinders quenching. A multi-phase constitutive model is employed for its modeling and simulation. Experimental analysis related to temperature evolution during the process and its resulting microstructure is developed and is used as a reference for the modeling effort. The kinetics of the diffusive transformations is described by *JMAK* (Johnson, Mehl, Avrami and Kolmogorov) law (Avrami, 1940; Cahn, 1956), while non-diffusive transformations are described by Koistinen-Marburger law. The energy equation thermomechanical coupling terms are analyzed considering two different models. The first one is an uncoupled model where thermomechanical terms are neglected, corresponding to the rigid body energy equation. The second model considers the latent heat associated with phase transformation in order to represent thermomechanical coupling. This second model is a first approach to represent 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.*, 2004).

A numerical procedure is developed based on the operator split technique (Ortiz *et al.*, 1983) associated with an iterative numerical scheme in order to deal with non-linearities in the formulation. With this assumption, the coupled governing equations are solved from four uncoupled problems: thermal, phase transformation, thermoelastic and elastoplastic. The proposed general formulation is applied to the through hardening of steel cylinders. Numerical results show that the proposed model is capable of capturing the general behavior observed on experimental data. Besides, numerical results present a good agreement with those of experimental data (Oliveira *et al.*, 2003), indicating some situations where it is important to consider the thermomechanical coupling terms.

2. PHENOMENOLOGICAL ASPECTS OF PHASE TRANSFORMATIONS

In quenching process, a steel piece is heated and maintained at constant temperature until austenite is obtained. Afterwards, a cooling process promotes the transformation of austenite phase into different phases and constituents which results in microstructures as: ferrite, cementite, pearlite, upper bainite, lower bainite and martensite. It can be observed that the microstructure of carbon alloy steel, depending on its chemical composition, can be composed by phases (austenite, ferrite, cementite and martensite) and constituents (pearlite, upper bainite and lower bainite). In order to describe all these microstructures in a macroscopically point of view, the volumetric fraction of each one of the phases and constituents of these microstructures is represented by β_i (austenite $i = A$ or 0, ferrite $i = 1$, cementite $i = 2$, pearlite $i = 3$, upper bainite $i = 4$, lower bainite $i = 5$ and martensite $i = M$ or 6). All of these microstructural constituents and phases may coexist, satisfying the following constraints: $\beta_A + \beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_M = 1$ and $0 \le \beta_i \le 1$.

Phase transformation from austenite to martensite is a non-diffusive transformation, which means that amount of volumetric phase is only a function of temperature (Chen *et al.*, 1997; Çetinel *et al.*, 2000; Reti *et al.*, 2001). This process may be described by the equation proposed by Koistinen and Marburger (1959) and the evolution of martensitic phase can be written in a rate form as follows (Oliveira *et al.*, 2003):

$$\dot{\beta}_M\left(T,\dot{T}\right) = \varsigma_{A\to M}\ \beta_A^0\left[\left(1-\beta_M\right)\left(k\dot{T}\right)\right] \quad ; \quad \varsigma_{A\to M}\left(\dot{T},T\right) = \Gamma\left(-\dot{T}\right)\Gamma\left(M_s - T\right)\Gamma\left(T - M_f\right) \tag{1}$$

where β_A^0 is the amount of austenite at the beginning of transformation, k is a material property, T is the temperature and $\Gamma(x)$ is the Heaviside function. Under a stress-free state, M_s and M_f are the temperatures where martensitic transformation starts and finishes its formation.

Pearlite, cementite, ferrite and bainite formations are diffusion-controlled transformation, which means that they are time dependent. The evolution of these phase transformations can be predicted through an approximate solution using data from Time-Temperature-Transformation diagrams (*TTT*) (Çetinel *et al.*, 2000; Reti *et al.*, 2001) and considering that the cooling process may be represented by a curve divided in a sequence of isothermal steps where the phase evolution is calculated considering isothermal transformation kinetics expressed by a *JMAK* law (Avrami, 1940; Cahn, 1956; Çetinel *et al.*, 2000; Reti *et al.*, 2001). The rate form of volumetric phase i can be written as follows (Oliveira *et al.*, 2003):

$$\dot{\beta}_r = \varsigma_{A\to phase(i)}\left\{ N_i(b_i)^{(1/N_i)}\left(\hat{\beta}_i^{\max} - \beta_i\right)\left[\ln\left(\frac{\hat{\beta}_i^{\max}}{\hat{\beta}_i^{\max} - \beta_i}\right)\right]^{\left(1-\frac{1}{N_i}\right)}\right\} \quad \left(i = 1,2,3,4,5\right); \tag{2}$$

where N_i is the Avrami exponent and b_i is a parameter that characterizes the rate of nucleation and growth processes (Avrami, 1940; Reti *et al.*, 2001). $\hat{\beta}_i^{\max} = \beta_i^{\max}\left[\sum_{j=1;\, j\neq i}^{5}\beta_j - \beta_M\right]$ (i = 1, ..., 5) where $\beta_i^{\max}$ represents the maximum volumetric fraction for a phase i and $\varsigma_{A\to phase(i)}\left(\dot{T},t\right) = \Gamma\left(-\dot{T}\right)\Gamma\left(t_i^f - t\right)\Gamma\left(t - t_i^s\right)$.

3. CONSTITUTIVE MODEL

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.*, 2001).

The phenomenological quenching model here proposed allows one to identify different aspects related to quenching process. With this aim, a Helmholtz free energy is proposed as a function of observable variables, total strain, ε_{ij}, and temperature, T. Moreover, the following internal variables are considered: plastic strain, ε_{ij}^{p}, volumetric fractions of seven different microstructures are considered: β_0, β_1, β_2, β_3, β_4, β_5, β_6 where $\beta_0 = \beta_A$ and $\beta_6 = \beta_M$. A variable related to kinematic hardening, α_{ij}, is also considered.

With these assumptions, the Helmholtz free energy function is defined as follows (assuming that β represents all β_i):

$$\rho\psi(\varepsilon_{ij},\varepsilon_{ij}^{p},\alpha_{ij},\beta,T) = W(\varepsilon_{ij},\varepsilon_{ij}^{p},\alpha_{ij},\beta,T) = W_e(\varepsilon_{ij}-\varepsilon_{ij}^{p},\beta,T) + W_\alpha(\alpha_{ij}) + W_\beta(\beta) - W_T(T) \tag{3}$$

where ρ is the material density. The elastic strain is defined as follows, assuming additive decomposition:

$$d\varepsilon_{ij}^{e} = d\varepsilon_{ij} - d\varepsilon_{ij}^{p} - \alpha_T dT\delta_{ij} - d\varepsilon_{ij}^{tv} - d\varepsilon_{ij}^{tp} \tag{4}$$

Equation (4) defines the elastic strain (left hand side). In the right hand side of this expression, the first term is the total strain while the second is related to plastic strain. The third term is associated with thermal expansion. The parameter α_T is the coefficient of linear thermal expansion, δ_{ij} is the Kronecker delta. The fourth term is related to volumetric expansion associated with phase transformation from a parent phase $d\varepsilon_{ij}^{tv} = (\sum_{r=1}^{6}\gamma_r d\beta_r)\delta_{ij}$, where γ_r is a material phase property related to total expansion. Finally, the last term is denoted as transformation plasticity strain $d\varepsilon_{ij}^{tp} = \sum_{r=1}^{6}\frac{3}{2}\kappa_r\, f'(\beta_r)d\beta_r\,\sigma_{ij}^{d}$, being the result of several physical mechanisms related to local plastic strain promoted by the phase transformation (Denis *et al.*, 1985; Sjöström, 1985); κ_r is a material phase parameter, $f(\beta_r)$ expresses the transformation process dependence and σ_{ij}^{d} the deviatoric stress defined by $\sigma_{ij}^{d} = \sigma_{ij} - \delta_{ij}(\sigma_{kk}/3)$, with σ_{ij} being the stress tensor component. It should be emphasized that this strain may be related to stress states that are inside the yield surface.

In order to describe dissipation processes, it is necessary to introduce a potential of dissipation or its dual $\phi^*(P_{ij}, X_{ij}, B^{\beta}, g_i)$, where P_{ij}, X_{ij}, B^{β}, g_i are thermodynamics forces associated with state variables $(\varepsilon_{ij},\varepsilon_{ij}^{p},\alpha_{ij},\beta,T)$.

By assuming that the specific heat is $c = -(T/\rho)\,\partial^2 W/\partial T^2$ and the set of constitutive equations (4-9), the energy equation can be written as (Pacheco, 1994):

$$\frac{\partial}{\partial x_i}\left(\Lambda\,\frac{\partial T}{\partial x_i}\right) - \rho c\dot{T} = -a_I - a_T \quad ; \quad \begin{cases} a_I = \sum_{r=1}^{6} B^{\beta_r}\dot{\beta}_r - X_{ij}\dot{\varepsilon}_{ij}^{p} + \sigma_{ij}\left(\dot{\varepsilon}_{ij}^{p} + \dot{\varepsilon}_{ij}^{tv} + \dot{\varepsilon}_{ij}^{tv}\right) \\ a_T = T\left[\frac{\partial\sigma_{ij}}{\partial T}\left(\dot{\varepsilon}_{ij} - \dot{\varepsilon}_{ij}^{p} - \dot{\varepsilon}_{ij}^{tp} - \dot{\varepsilon}_{ij}^{tv}\right) - \sum_{r=1}^{6}\frac{\partial B^{\beta_r}}{\partial T}\dot{\beta}_r + \frac{\partial X_{ij}}{\partial T}\dot{\varepsilon}_{ij}^{p}\right] \end{cases} \tag{5}$$

Terms a_I and a_T are, respectively, internal and thermal coupling. The first one is always positive and has a role in the energy equation similar to a heat source in the classical heat equation for rigid bodies. The thermomechanical coupling effect related to phase transformation may be represented as a latent heat released during the phase transformation (Fernandes *et al.*, 1985; Denis *et al.*, 1987; Woodard *et al.*, 1999): $a_I + a_T = \dot{Q} = \sum_{i=1}^{6}\Delta H_i\,\dot{\beta}_i$ where ΔH_i is the enthalpy variation in a transformation process involving a previous phase (austenite) and a product phase β_i (i = 1,…,6). Therefore, this source term is used instead of thermomechanical coupling terms, which represents a first approach of the general formulation (Silva *et al.*, 2004). It should be notice that the energy conservation problem considers either convection or radiation as boundary conditions.

4. CYLINDRICAL BODIES

This contribution considers cylindrical bodies as an application of the proposed general formulation. With this assumption, heat transfer analysis may be reduced to a one-dimensional problem. Moreover, plane stress or plane strain state can be assumed. Under these assumptions, only radial, r, circumferential, θ, and longitudinal, z, components need to be considered and a one-dimensional model is formulated. For this case, tensor quantities presented in the previous section may be replaced by scalar or vector quantities. As examples, one could mention: E_{ijkl} replaced by E; H_{ijkl} replaced by H; σ_{ij} replaced by σ_i (σ_r , σ_θ , σ_z). The second one is an axisymmetric finite element model and can be used to study more complex geometries like notched cylinders. A detailed description of these simplifications could be found in Pacheco *et al.* (2001), Silva *et al.* (2004, 2005) and Oliveira *et al.* (2003).

The numerical procedure here proposed is based on the operator split technique (Ortiz *et al.*, 1983; Pacheco, 1994) associated with an iterative numerical scheme in order to deal with non-linearities in the formulation. With this assumption, coupled governing equations are solved from four uncoupled problems: thermal, phase transformation, thermo-elastic and elastoplastic.

Thermal Problem - Comprises a radial conduction problem with convection. Material properties depend on temperature, and therefore, the problem is governed by non-linear parabolic equations. An implicit finite difference predictor-corrector procedure is used for numerical solution (Ames, 1992; Pacheco, 1994).

Phase Transformation Problem – The volumetric fractions of the phases are determined in this problem. Evolution equations are integrated from a simple implicit Euler method (Ames, 1992; Nakamura, 1993).

Thermo-elastic Problem - Stress and displacement fields are evaluated from temperature distribution. Numerical solution is obtained employing a shooting method procedure (Ames, 1992; Nakamura, 1993).

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 (Simo & Hughes, 1998).

5. EXPERIMENTAL PROCEDURE

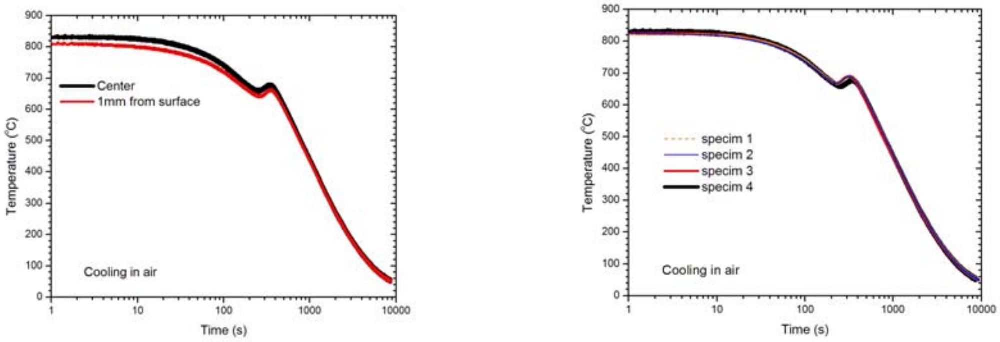
The experimental procedure adopted consists of heating cylindrical specimens with external radius R = 25.4 mm = 1”, made by SAE 4140H, in a furnace to a suitable austenitizing temperature (830°C), holding at that temperature for a sufficient time to promote the desired change in crystalline structure in all parts of the workpiece (1 hour), and finally cooling in two different media: air and water. Four cylindrical specimens are used: one specimen with two holes (one at the cylinder center and the other at 1 mm from the cylinder surface) and three other specimens with one hole at the cylinder center. Thermocouples are introduced at each hole and the temperature time history is acquired and registered by a data acquisition system. Figure 1 shows the furnace, the data acquisition system and the cylindrical specimen (Oliveira *et al.*, 2003; Oliveira, 2004).

(*a*) (*b*) (*c*)

Figure 1 - (*a*) Furnace, (*b*) data acquisition system and (c) cylindrical specimen.

5.1. Air Cooling

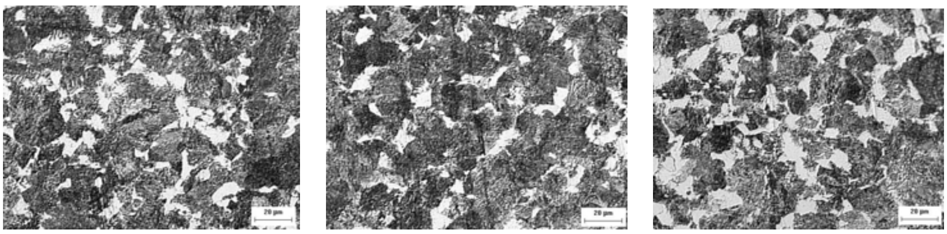
At first, air cooling medium is of concern. Figure 2 presents the temperature time history curves. Figure 2*a* presents the thermocouple response at the specimen center and also at 1 mm from the cylinder surface. On the other hand, Fig. 2*b* shows the response from different specimens where the thermocouple is at the cylinder center. It should be pointed out that, when the specimen is about 650°C, a temperature increase can be observed. This phenomenon is related to the thermomechanical coupling (Silva *et al.*, 2004; Denis, 1996; Woodard *et al.*, 1999) associated with the latent heat of the austenite $\rightarrow$ pearlite phase transformation.



(*a*) (*b*)

Figure 2 – (*a*) Air cooling temperature evolution at the center and at 1 mm from the cylinder surface. (*b*) Temperature time history from four specimens measured at the cylinder center.

Figure 3 presents the microstructure at an internal cross section of the cylinder far from the edges, at three regions ($r = 0$, $r = 0.5\,R$ and $r = R$). The metallographic analysis developed reveals a homogeneous radial phase distribution with 24% of ferrite and 76% of pearlite.

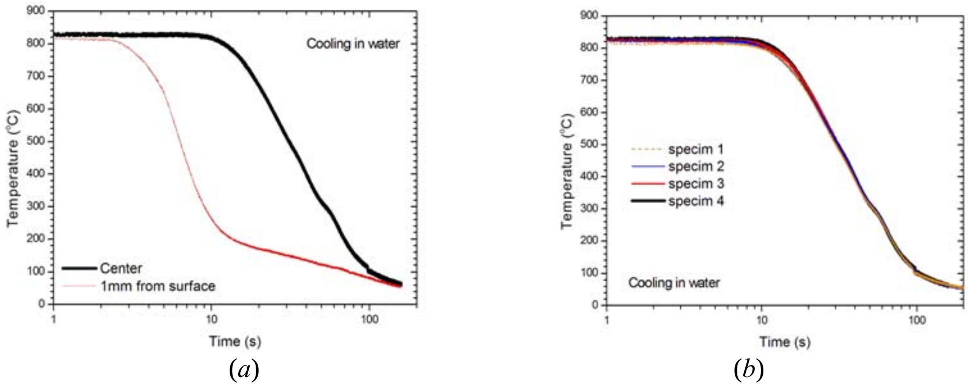


(*a*) (*b*) (*c*)

Figure 3 – Air cooling specimen microstructure: (*a*) center ($r = 0$), (*b*) $r = 0.50R$ and (*c*) surface ($r = R$).

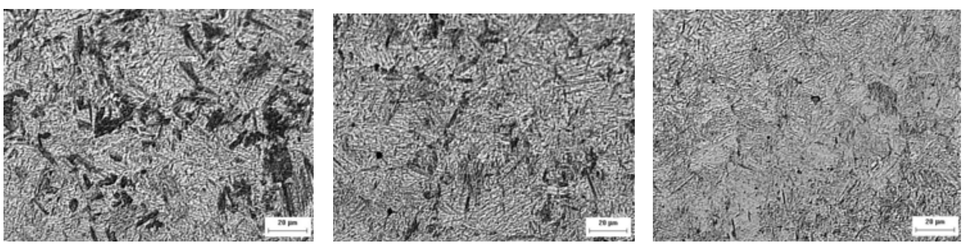
5.2. Water Cooling

At this point, water cooling medium is considered. This is related to a severe quenching and it is expected a great level of matensitic formation. Figure 4 presents the temperature time history curves while Fig. 5 presents the metallographic analysis. The metallographic analysis developed reveals a homogeneous radial phase distribution with 100% of martensite after the quenching process.



(*a*) (*b*)

Figure 4 - (*a*) Temperature time history at the center and at 1 mm from the surface for the cylinders. (*b*) Temperature time history for four specimens cooled in water.



(*a*) (*b*) (*c*)

Figure 5 – Water cooling specimen microstructure: (*a*) center ($r = 0$), (*b*) $r = 0.50R$ and (*c*) suface ($r = R$).

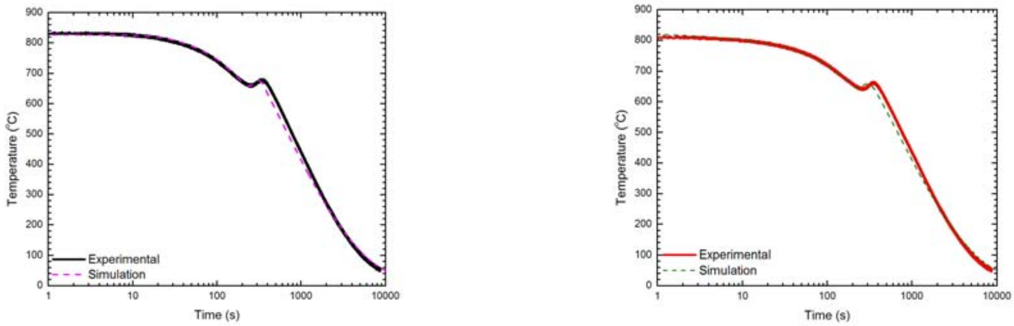
6. NUMERICAL RESULTS: MODEL VERIFICATION

The forthcoming analysis tries to reproduce the conditions of the experiment described in the last section using numerical simulations related to the developed model for the two quenching processes discussed: air and water cooling. Therefore, a SAE 4140H, 1" radius cylinder quenched in air and water are considered.

Material parameters of the SAE 4140H are the following (Denis *et al.*, 1985, 1999; Woodard, *et al.*, 1999; Sjöström, 1985; Melander, 1985; Oliveira, 2004): γ_1 = 3.333 × 10-3, γ_2 = 0, γ_3 = γ_4 = γ_5 = 5.000 × 10–3, γ_6 = 1.110×10–2, $\kappa_i = \left[5/\left(2\sigma_Y^o\right)\right]\gamma_i$ (where σ_Y^o is the austenite yielding stress and $i = 1,...,6$), $\rho = 7.800 \times 10^3\, kg/m^3$, $M_s = 340°C$, $M_f = 140°C$. Other parameters depend on temperature and needs to be interpolated from experimental data. Therefore, parameters $E^i, H^i, \sigma_Y^i, \alpha_T^i, c^i, \Lambda^i$, where $i = 1,...,6$, and the convection coefficient, *h*, are evaluated by polynomial expressions (Melander, 1985; Hildenwall, 1979; Pacheco *et al.*, 2001; Silva *et al.*, 2004). Temperature dependent parameters for diffusive phase transformations are obtained from TTT diagrams (ASM, 1977). Moreover, latent heat released associated with the enthalpy variation in a transformation process involving a parent phase (austenite) and a product phase β_i are given by: $\Delta H_1 = 1.55 \times 10^9 - 2.31 \times 10^4 T + 15.97 T^2 - 4.29 \times 10^{-3} T^3 - 5.00 \times 10^9 / T$ J/m^3, $\Delta H_3 = 1.56 \times 10^9 - 1.5 \times 10^6 T \quad J/m^3$, $\Delta H_6 = 640 \times 10^6 \quad J/m^3$ (Denis *et al.*, 1987; Woodard *et al.*, 1999).

6.1. Air Cooling

In order to compare numerical and experimental results, it is presented in Fig. 6 the temperature time history in two different positions: at the center and at 1 mm from the surface for the cylinder. It is noticeable the close agreement between results and it is important to highlight that the thermomechanical coupling effect is captured by the model.



(*a*) (*b*)

Figure 6 - Air cooling temperature time history: (a) at the center and (b) at 1 mm from the cylinder surface.

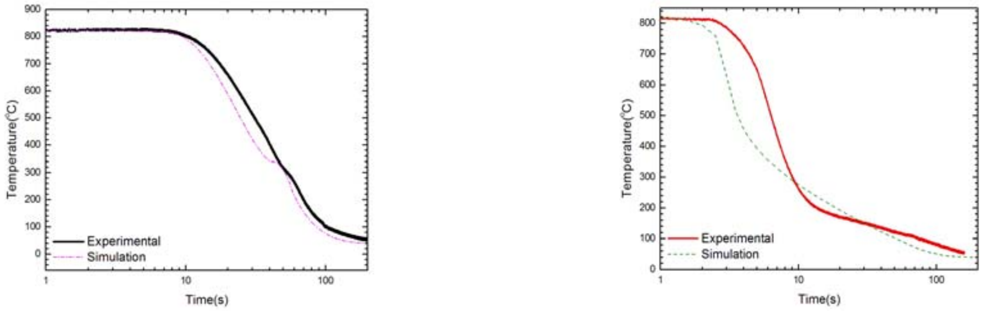
Based on numerical simulations, it is evaluated the volume fraction distribution. Results are summarized in Tab. 1, showing again, a close agreement with experimental results presented in Section 5.1.

Table 1 – Air cooling simulation: Volumetric fraction phase distribution.

Phase	**Volumetric Fraction (%)**		
	r = 0	*r* = 0.50*R*	*r* = *R*
Austenite	0	0	0
Ferrite	27	27	27
Pearlite	73	73	73
Bainite	0	0	0
Martensite	0	0	0

6.2. Water Cooling

The quenching process in water is now in focus. Temperature time history in two different positions (at the cylinder center and at 1 mm from the cylinder surface) are presented in Fig. 7. At the body center there is a close agreement between numerical and experimental results. By considering the position at 1mm from the surface, on the other hand, results capture just the general behavior. This discrepancy is explained by the thermocouple influence. Actually, it is possible to make adjustments considering the heat conduction through the thermocouple and evaluating the temperature at its center. The finite element method may be used with this aim. The commercial code ANSYS is employed in order to evaluate the temperature distribution measured at the thermocouple center. Element PLANE13 is employed and results are presented in Fig. 8 showing a good agreement with experimental results.



(*a*) (*b*)

Figure 7 - Air cooling temperature time history: (a) at the center and (b) at 1 mm from the surface for the cylinders.

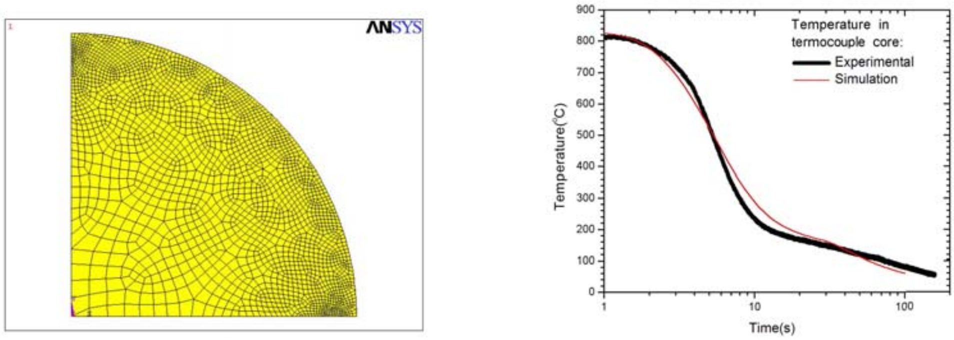


Figure 8 – Finite element simulation considering temperature at the thermocouple center.

Based on numerical simulations, it is evaluated the volume fraction distribution, summarized in Tab. 2. Now, numerical results still in agreement with experimental data, however, simulations had predicted the presence of bainite in contrast with experiment. Nevertheless, it is important to observe that experimental data uses optical analysis in order to conclude the phase distribution and therefore, this difference may be less than presented.

Table 2 – Water cooling simulation: Volumetric fraction phase distribution.

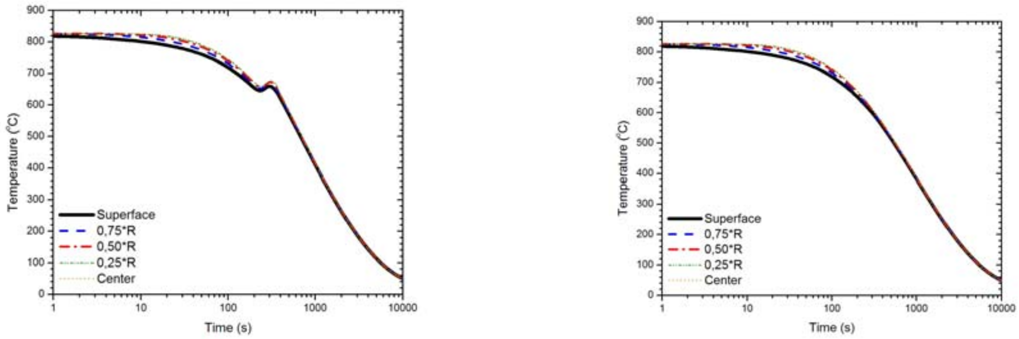
Phase	**Volumetric Fraction (%)**		
	$r = 0$	$r = 0.50R$	$r = R$
Austenite	0	0	0
Ferrite	0	0	0
Pearlite	0	0	0
Bainite	11	11	0
Martensite	89	89	100

7. NUMERICAL RESULTS: THERMOMECHANICAL COUPLING INFLUENCE

After the verification of the model capacity to capture the general behavior of quenching process, some numerical simulations are performed in order to evaluate the effect of thermomechanical coupling in the process modeling. Two models are considered with this aim: *coupled* and *uncoupled*. The *coupled* model considers the latent heat associated with phase transformation as a source in the energy equation, which results are in close agreement with those obtained from experimental tests. The *uncoupled* model, on the other hand, neglects the thermomechanical couplings, corresponding to the rigid body energy equation. Once again, two different processes are of concern: air and water cooling.

7.1. Air Cooling

This section treats numerical simulations related to the quenching process in air. Temperature time history for the two models for five positions of the cylinder is now considered (Fig. 9). As expected, the *coupled* model shows the temperature increase at about 650°C at all the five positions, which is associated with the latent heat of the austenite → pearlite phase transformation. The *uncoupled* model, on the other hand, does not captures this phenomenon observed in experimental data.



(*a*) (*b*)

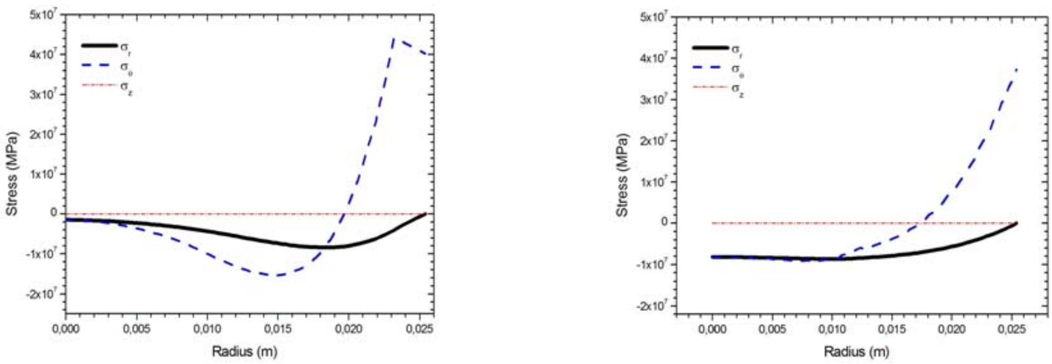
Figure 9 - Temperature time history for (*a*) *coupled* and (*b*) *uncoupled* models.

The phase distribution along the cylinder radius for both models is analyzed with the aid of Tab. 3. It can be observed that in contrast of the prediction of the *coupled* model, which is in close agreement with the experimental data, the *uncoupled* model does not fit the experimental data and upper bainite is predicted together with ferrite and pearlite. The formation of bainite (observed only on the *uncoupled* model prediction) is related to the faster cooling rate. Notice that the temperature time history observed in experimental data and also in numerical results predicted by the *coupled* model presents a temperature rise near 650°C which delays the cooling and avoids the bainitic formation.

Table 3 - Volumetric phase distribution for *coupled* and *uncoupled* models.

Phase	*Coupled Model*			Phase	*Uncoupled Model*		
	$r = 0$	$r = 0.50R$	$r = R$		$r = 0$	$r = 0.50R$	$r = R$
Austenite	0	0	0	Austenite	0	0	0
Ferrite	27	27	27	Ferrite	26	27	27
Pearlite	73	73	73	Pearlite	71	73	73
Bainite	0	0	0	Bainite	3	0	0
Martensite	0	0	0	Martensite	0	0	0

The residual stress distribution along the cylinder radius for both models is presented Fig. 10. In spite of the low values of stresses observed, a comparison between numerical results show that the thermomechanical coupling affects the stress distribution.

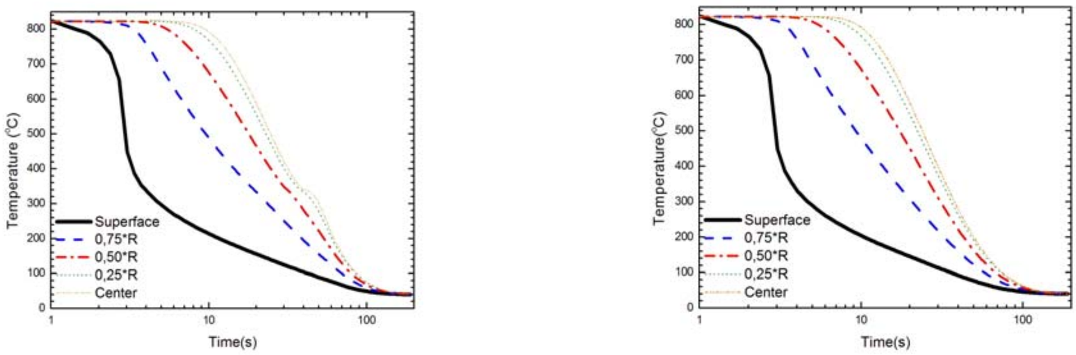


(*a*) (*b*)

Figure 10 – Residual stress distribution for (*a*) *coupled* and (*b*) *uncoupled* models.

7.2 - Water Cooling

At this point, quenching in water is in focus. Temperature time history for the two models for five positions of the cylinder is presented in Fig. 11. In contrast with results related to air cooling, these results are essentially the same.



(*a*) (*b*)

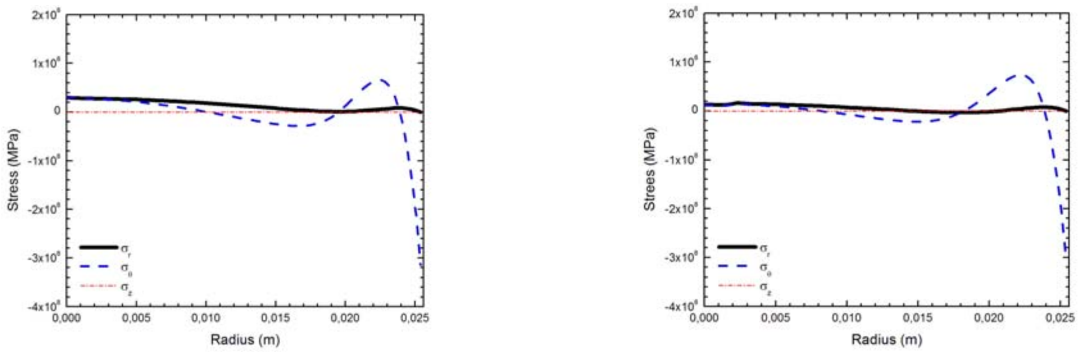
Figure 11 - Temperature time history for (*a*) *coupled* and (*b*) *uncoupled* models.

The phase distribution along the cylinder radius for both models is analyzed with the aid of Tab. 4.

Table 4 - Volumetric phase distribution for *coupled* and *uncoupled* models.

Phase	*Coupled Model*			Phase	*Uncoupled Model*		
	r = 0	*r* = 0.50*R*	*r* = *R*		*r* = 0	*r* = 0.50*R*	*r* = *R*
Austenite	0	0	0	Austenite	0	0	0
Ferrite	0	0	0	Ferrite	0	0	0
Pearlite	0	0	0	Pearlite	0	0	0
Bainite	11	11	0	Bainite	11	11	3
Martensite	89	89	100	Martensite	89	89	97

Figure 12 shows the residual stress distribution along the cylinder radius for both models. In spite of the low values of stress observed, a comparison between numerical results show that the thermomechanical coupling does not affect significantly the stress distribution.



(*a*) (*b*)

Figure 12 – Residual stress distribution for (*a*) *coupled* and (*b*) *uncoupled* models.

8. CONCLUSIONS

The present contribution discusses the thermomechanical analysis of quenching process. Modeling and simulation are developed from an anisothermal multi-phase constitutive model formulated within the framework of continuum mechanics and thermodynamics of irreversible processes. This approach allows a direct extension to more complex situations, as the analysis of three-dimensional media. A numerical procedure is developed based on the operator split technique associated with an iterative numerical scheme in order to deal with non-linearities in the formulation. The proposed numerical procedure allows the use of traditional numerical methods, like the finite element method. Through hardening of cylindrical bodies is considered as application of the proposed general formulation. Two different cooling media are of concern: air and water. An experimental procedure is developed to evaluate the temperature history during the process and the phase distribution at the end of the process. Numerical simulations present a good agreement with experimental data, indicating some situations where it is important to consider the energy equation thermomechanical coupling terms, represented by the latent heat associated with phase transformation as a source term. Results related to air cooling shows that thermomechanical couplings are very important. On the other hand, thermomechanical couplings do not have significant influence on water cooling process.

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10. REFERENCES

Ames, W. F., 1992, "*Numerical Methods for Partial Differential Equations*", Academic Press.

ASM, 1977, *"Atlas of Isothermal Transformation and Cooling Transformation Diagrams"*, American Society Metals.

Avrami, M., 1940, "Kinetics of Phase Change. II: Transformation-Time relations for random distribution of nuclei", *Journal of Chem. Phys.*, v.8, pp.212.

Cahn, J. W., 1956, "Transformation Kinetics During Continuous Cooling", *Acta Metallurgica*, v.4, pp.572-575.

Çetinel, H., Toparlı, M. & Özsoyller, 2000, "A Finite Element Based Prediction of the Microstructural Evolution of Steels Subjected to the Tempcore Process", *Mechanics of Materials*, v.32, pp.339-347.

Chen, J. R., Tao, Y. Q. & Wang, H.G., 1997, "A Study on Heat Conduction with Variable Phase Transformation Composition during Quench Hardening", *Journal of Materials Processing Technology*, v.63, pp.554-558.

Denis S., 1996, "Considering Stress-Phase Transformation Interaction in the Calculation of Heat Treatment Residual Stresses", Journal de Physique IV, v.6, January, pp.159-174.

Denis, S., Gautier, E., Simon, A. & Beck, G., 1985, "Stress-Phase-Transformation Interactions – Basic Principles, Modelling and Calculation of Internal Stresses", *Material Science and Technology*, v.1, October, p.805-814.

Denis, S., Sjöström, S. & Simon, A., 1987, "Coupled Temperature, Stress, Phase Transformation Calculation Model Numerical Illustration of the Internal Stresses Evolution during Cooling of a Eutectoid Carbon Steel Cylinder", *Metallurgical Transactions A*, v.18A, July, pp.1203-1212.

Denis, S., Archambault, S., Aubry, C., Mey, A., Louin, J. C. & Simon, A., 1999, "Modelling of Phase Transformation Kinetics in Steels and Coupling with Heat Treatment Residual Stress Predictions", *Journal de Physique IV*, v.9, September, pp.323-332.

Fernandes, M. B., Denis, S. & Simon, A., 1985, "Mathematical Model Coupling Phase Transformation and Temperature Evolution during Quenching of Steels", Materials Science and Technology, v.1, October, pp.838-844.

Hildenwall, B., 1979, "*Prediction of the Residual Stresses Created During Quenching*", Ph.D. Thesis, Linkoping Univ.

Hömberg, D., 1996, "A Numerical Simulation of the Jominy End-quench Test", *Acta Mater.*, v.44, n.11, pp.4375-4385

Inoue, T. & Wang, Z., 1985, "Coupling between Stress, Temperature, and Metallic Structures during Processes Involving Phase Transformations", *Material Science and Technology*, v.1, pp.845-850.

Koistinen, D. P. & Marburger, R. E., 1959, "A General Equation Prescribing the Extent of the Austenite-Martensite Transformation In Pure Iron-Carbon Alloys and Plain Carbon Steels", *Acta Metallurgica*, v.7, pp.59-60.

Lemaitre, J. & Chaboche, J.L., 1990, *"Mechanics of Solid Materials"*, Cambridge Press Univ.

Melander, M., 1985, "*A Computational and Experimental Investigation of Induction and Laser Hardening*", Ph.D. Thesis, Department of Mechanical Eng., Linkoping University.

Nakamura, S., 1993, "*Applied Numerical Methods in C"*, Prentice-Hall.

Ortiz, M., Pinsky, P. M. & Taylor, R. L., 1983, "Operator Split Methods for the Numerical Solution of the Elastoplastic Dynamic Problem", *Computer Methods in Applied Mechanics and Engineering*, v.39, pp.137-157.

Oliveira, W. P., Souza, L. F. G., Pacheco, P. M. C. L. & Savi, M. A., 2003, "Quenching Process Modeling in Steel Cylinders Using a Multi-Phase Constitutive Model", *COBEM 2003 - 17th International Congress of Mechanical Engineering*, São Paulo.

Pacheco, P. M. C. L., 1994, *"Analysis of Thermomechanical Coupling in Elasto-viscous-plastic Materials"*, Ph.D. Thesis, Department of Mechanical Engineering, PUC-Rio.

Pacheco, P. M. C. L., Savi, M. A. & Camarão, A. F., 2001, "Analysis of Residual Stresses Generated by Progressive Induction Hardening of Steel Cylinders", *Journal of Strain Analysis for Engineering Design*, v.36, n.5, pp.507-516.

Reti, T., Fried, Z. & Felde, I., 2001, "Computer Simulation of Steel Quenching Process using a Multi-Phase Transformation Model", *Computational Materials Science*, v.22, pp.261-278.

Sen, S., Aksakal, B. & Ozel, A., 2000, "Transient and Residual Thermal Stresses in Quenched Cylindrical Bodies", *International Journal of Mechanical Sciences*, v.42 n.10, p.2013-2029.

Silva, E. P., Pacheco, P. M. C. L. & Savi, M. A., 2003, "Simulation of Quenching Process Using the Finite Element Method", *COBEM 2003 - 17th International Congress of Mechanical Engineering*.

Silva, E. P., Pacheco, P. M. C. L. & Savi, M. A., 2004, "On the Thermo-Mechanical Coupling in Austenite-Martensite Phase Transformation Related to the Quenching Process", *International Journal of Solids and Structures*, v.41, n.3-4, pp.1139-1155.

Silva, E. P., Pacheco, P. M. C. L. & Savi, M. A., 2005, "Finite Element Analysis of the Phase Transformation Effect in Residual Stresses Generated by Quenching in Notched Steel Cylinders", *Journal of Strain Analysis for Engineering Design*, v.40, n.2, p.151-160.

Simo, J. C. & Hughes, T. J. R., 1998, "*Computational Inelasticity*", Springer.

Sjöström, S., 1985, "Interactions and Constitutive Models for Calculating Quench Stresses in Steel", *Material Science and Technology*, v.1, p.823-829.

Woodard, P. R., Chandrasekar, S. & Yang, H. T. Y., 1999, "Analysis of Temperature and Microstructure in the Quenching of Steel Cylinders", *Metallurgical and Materials Trans. B-Process Metallurgy and Materials Processing Science*, v.4, August, p.815-822.

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