ON THE PHASE TRANSFORMATION EFFECT IN RESIDUAL STRESSES GENERATED BY QUENCHING IN NOTCHED STEEL CYLINDERS

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Abstract. *The determination of residual stresses is an important task in the analysis of quenching process. Nevertheless, due to the complexity of the phenomenon, many simplifications are usually adopted in the prediction of these stresses for engineering purposes. One of these simplifications is the effect of phase transformation. Many studies analyse residual stresses generated by quenching process considering a thermo-elastoplastic approach, neglecting phase transformation. The present study analyses the effect of austenite-martensite phase transformation during quenching in the determination of residual stresses, comparing two different models: complete (thermo-elastoplastic model with austenite-martensite phase transformation) and without phase transformation (thermo-elastoplastic model without phase transformation). The finite element method is employed for spatial discretization together with a constitutive model that represents the thermomechanical behaviour of the quenching process. Progressive induction hardening of steel cylinders with semi-circular notches is of concern. Numerical simulations show situations where great discrepancies are introduced in the predicted residual stresses if phase transformation is neglected.*

Keywords: *Quenching, Phase transformation, Thermomechanical coupling, Finite Element.*

1. Introduction

Considerable residual stresses may arise during quenching process and therefore, their prediction is an important task (Denis *et al.*, 1985, Denis *et al.*, 1999, Woodard *et al.*, 1999, Sjöström, 1985, Sen *et al.*, 2000). Since phenomenological aspects of quenching involve couplings among different physical phenomena, their description is unusually complex. Moreover, engineering purposes usually introduces many simplifications in order to predict residual stresses generated during quenching. Neglecting the phase transformations is one of these simplifications in the modelling of the quenching process.

Sen *et al.* (2000) consider steel cylinders without phase transformations. Other authors analyse simple geometries incorporating the effect of phase transformations (Çetinel *et al.*, 2000, Gür and Tekkaya, 2001, Chen *et al.*, 1997, Gür and Tekkaya, 1996). There are also some other complex aspects related to quenching that could be incorporated in the modelling of this process. As example, one can cite the heat generated during phase transformation, usually treated by considering the latent heat associated with phase transformation (Denis *et al.*, 1999, Inoue 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 usually treated in literature and their analysis is an important topic to be investigated (Silva *et al.*, 2004).

The present contribution concerns with the importance of phase transformation in the analysis of residual stresses generated by the quenching process. On this basis, simulations of two different models are carried out: *complete* (thermo-elastoplastic model with austenite-martensite phase transformation) and *without phase transformation* (thermo-elastoplastic model without phase transformation). The finite element method associated with a constitutive model proposed by Pacheco *et al.* (2001a-b) and Silva *et al.* (2004) is considered. The constitutive model describes the thermomechanical behaviour related to the quenching process considering different phenomenological phenomena as the plasticity with kinematic hardening, the thermal expansion, the austenite-martensite phase transformation and some related aspects associated with this phase transformation as the volumetric expansion and the transformation plasticity. This anisothermal model is formulated within the framework of continuum mechanics and the thermodynamics of irreversible processes and captures the general behaviour of quenching (Silva *et al.*, 2004, Pacheco *et al.*, 2001a-b). Numerical procedures described in Silva (2002) are employed in order to deal with nonlinearities of the formulation.

In this contribution, as an application of the general procedure, progressive induction hardening of steel cylinder bodies is analysed. Since mechanical components usually have geometric discontinuities that promote local perturbations in the variables distribution, it is important to consider this type of perturbation in the analysis. Here, this perturbation is contemplated introducing a semi-circular notch in the steel cylinder. Numerical simulations show situations where great discrepancies are introduced in the predicted residual stresses neglecting phase transformation.

2. Constitutive Model

This contribution describes the quenching process with the aid of a constitutive model presented in Pacheco *et al.* (2001a-b) and Silva *et al.* (2004). This model is formulated within the framework of continuum mechanics and the thermodynamics of irreversible processes. Here, a brief description of this model is presented and a detailed explanation may be found in references (Silva *et al.*, 2004, Pacheco *et al.*, 2001a-b, Silva, 2002). Therefore, considering that ε_{ij} is the total strain, T, the temperature, ε_{ij}^p, the plastic strain, β, the volumetric fraction of martensitic phase, and α_{ij}, a variable related to kinematic hardening, the following constitutive relation may be written, denoting σ_{ij} as the stress tensor component:

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

where E_{ijkl} is associated with components of the elastic tensor and Φ_{ijpq} is an auxiliary tensor defined as the inverse of C_{ijpq}:

$$C_{ijpq} = \delta_{pi}\delta_{qj} + \frac{3}{2} E_{ijpq}\kappa\beta(2-\beta) \tag{2}$$

δ_{ij} is the Kronecker delta. The expression of the constitutive equation is obtained assuming an elastic strain with the form:

$$\varepsilon_{ij}^e = \varepsilon_{ij} - \varepsilon_{ij}^p - \alpha_T (T - T_0)\delta_{ij} - \gamma\beta\delta_{ij} - (3/2)\kappa\sigma_{ij}^d \beta(2-\beta)\,. \tag{3}$$

Observing the right hand of the equation, the third term, $\alpha_T (T - T_0)\delta_{ij}$, is associated with thermal expansion. The parameter α_T is the coefficient of linear thermal expansion and T_0 is a reference temperature. The fourth term, $\gamma\beta\delta_{ij}$, is related to volumetric expansion associated with phase transformation from austenite to martensite. Therefore, when part of a material experiences phase transformation, there is an increment of volumetric strain, proportional to γ, a material property related to the total expansion associated with martensitic transformation. Finally, the last term, $(3/2)\kappa\sigma_{ij}^d \beta(2-\beta)$, is denoted as transformation induced plasticity strain, being the result of several physical mechanisms (Denis *et al.*,1985, Sjöström, 1985). This behaviour is related to localized plastic strain promoted by the martensitic transformation. In this term, the deviatoric stress component is defined by $\sigma_{ij}^d = \sigma_{ij} - \delta_{ij}(\sigma_{kk}/3)$. Moreover, κ is a material parameter. It should be emphasized that this strain may be related to stress states that are inside the yield surface.

The evolution of internal variables is governed by the following equations:

$$\dot{\varepsilon}_{ij}^p = \lambda\, \mathrm{sign}\left(\sigma_{ij} - H_{ijkl}\alpha_{kl}\right) \tag{4}$$

$$\dot{\alpha}_{ij} = \dot{\varepsilon}_{ij}^p \tag{5}$$

$$\dot{\beta} = \varsigma_{A \to M}\, k\dot{T}(M_s - T)\exp\left[-k(M_s - T)\right] \tag{6}$$

where sign(x) = x / $|x|$ and λ is the plastic multiplier from the classical theory of plasticity. The term $H_{ijkl}\alpha_{kl} = X_{ij}$ is related to the kinematic hardening, where H_{ijkl} is the kinematic hardening modulus tensor. Phase transformation is described by the equation proposed by Koistinen and Marburger (1959) to express the kinetics of phase transformation from austenite to martensite. In this expression, k is a material constant and M_s is the temperature where martensite starts to form in the stress-free state. Moreover, the following expression is used in order to impose proper conditions to the phase transformation:

$$\varsigma_{A\to M}\left(\dot{T},T\right)=\Gamma\left(\left|\dot{T}\right|-rMs\right)\cdot\Gamma\left(M_s-T\right)\cdot\Gamma\left(T-M_f\right) \tag{7}$$

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. Moreover, $\Gamma(x)$ is the Heaviside function. The *von Mises* criterion is expressed by (Silva *et al.*, 2004),

$$f(\sigma_{ij},\alpha_{ij})=\left[\frac{3}{2}(\sigma_{ij}^d-X_{ij}^d)(\sigma_{ij}^d-X_{ij}^d)\right]^{1/2}-\sigma_Y\le 0 \tag{8}$$

here σ_Y is the yield stress and X_{ij}^d is the deviatoric part of X_{ij}, the kinematic hardening tensor, defined as follows:

$$X_{ij}^d = X_{ij} - \delta_{ij}\,(X_{kk}/3) \tag{9}$$

The description of thermal problem assumes classical energy equation for rigid bodies,

$$\frac{\partial}{\partial x_i}\left(\Lambda\frac{\partial T}{\partial x_i}\right)-\rho c\dot{T}=0 \tag{10}$$

where Λ is the coefficient of thermal conductivity, ρ is the density and c is the specific heat. Notice that terms related to thermomechanical coupling are neglected (Silva *et al.*, 2004).

These expressions provide a complete set of equations that describes the thermomechanical behaviour of solids during quenching process. Notice that it is a nonlinear set, being necessary proper numerical procedures to its solution.

3. Finite Element Model

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

Thermal Problem – Comprises conduction problem with 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 *et 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-b, 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 (Simo and Hughes, 1998).

As an application of the general procedure, axisymmetric triangular elements are adopted for all finite element moduli, considering classical shape functions (Segerlind, 1984). Besides, the original three-dimensional constitutive model is reduced to a simplified version in order to describe the quenching process in steel cylinders. With this assumption, heat transfer analysis may be reduced to a bi-dimensional problem and for the stress components only radial, r, tangential, θ, and axial, z, components need to be considered together with shear components $r\theta$. In brief, it is important to notice that tensor quantities may be replaced by scalar or vector quantities. As examples, one could mention: E_{ijkl} replaced by E; H_{ijkl} replaced by H; and non-vanishing components of σ_{ij} are σ_r, σ_θ, σ_z, σ_{rz}.

4. Numerical Simulations

In order to analyse the effect of phase transformation during quenching process, numerical investigations are carried out simulating a progressive induction (PI) hardening. PI hardening is a heat treatment process that is done moving a workpiece at a constant speed through a coil and a cooling ring. A hard surface layer with high compressive residual stresses, combined with a tough core with tensile residual stresses, is usually obtained.

This article considers PI hardening simulations in a long cylindrical SAE 4140H steel bar. Material parameters for numerical simulation are presented in Tab. 1. Other parameters depend on temperature and are interpolated from experimental data as follows (in SI units) (Silva *et al.*, 2004, Pacheco *et al.*, 2001a-b, Silva, 2002, Camarão, 1998, Melander, 1985a-b, Hildenwall, 1979, Camarão *et al.*, 2000):

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

$$E = E_A\,(1-\beta) + E_M\,\beta \qquad \begin{cases} E_A = 1.985\times10^{11} - 4.462\times10^{7}T - 9.909\times10^{4}T^{2} - 2.059T^{3} \\ E_M = 2.145\times10^{11} - 3.097\times10^{7}T - 9.208\times10^{4}T^{2} - 2.797T^{3} \end{cases} \tag{11}$$

$$H = \begin{cases} 2.092\times10^{8} + 3.833\times10^{7}T - 3.459\times10^{4}T^{2}, & \text{if } T \le 723K \\ 2.259\times10^{11} - 2.988\times10^{8}T, & \text{if } 723K < T \le 748K \\ 5.064\times10^{9} - 3.492\times10^{6}T, & \text{if } T > 748K \end{cases} \tag{12}$$

$$\sigma_Y = \begin{cases} 7.520\times10^{8} + 2.370\times10^{5}T - 5.995\times10^{2}T^{2}, & \text{if } T \le 723K \\ 1.598\times10^{10} - 2.126\times10^{7}T, & \text{if } 723K < T \le 748K \\ 1.595\times10^{8} - 1.094\times10^{5}T, & \text{if } T > 748K \end{cases} \tag{13}$$

$$\alpha_T = \begin{cases} 1.115\times10^{-5} + 1.918\times10^{-8}T - 8.798\times10^{-11}T^{2} + 2.043\times10^{-13}T^{3}, & \text{if } T \le 748K \\ 2.230\times10^{-5}, & \text{if } T > 748K \end{cases} \tag{14}$$

$$c = 2.159\times10^{2} + 0.548T \tag{15}$$

$$\Lambda = 5.223 + 1.318\times10^{-2}T \tag{16}$$

Heat transfer coefficient, *h*, for cooling fluid (Ucon E 2.8%) and air are respectively given by (in SI units) (Silva *et al.*, 2004, Pacheco *et al.*, 2001a-b, Silva, 2002, Camarão, 1998, Melander, 1985a-b, Hildenwall, 1979, Camarão *et al.*, 2000):

$$h = \begin{cases} 6.960\times10^{2}, & \text{if } T \le 404K \\ 2.182\times10^{4} - 1.030\times10^{2}T + 1.256\times10^{-1}T^{2}, & \text{if } 404K < T \le 504K \\ -2.593\times10^{4} + 5.500\times10^{2}T, & \text{if } 504K < T \le 554K \\ -9.437\times10^{4} + 4.715\times10^{2}T - 7.286\times10^{-1}T^{2} + 3.607\times10^{-4}T^{3}, & \text{if } 554K < T \le 804K \\ 1.210\times10^{3}, & \text{if } T > 804K \end{cases} \tag{17}$$

$$h_{air} = \begin{cases} 2.916 + 6.104\times10^{-2}T - 1.213\times10^{-4}T^{2}, & \text{if } T \le 533K \\ 6.832 + 1.837\times10^{-2}T - 1.681\times10^{-5}T^{2} + 6.764x10^{-9}T^{3}, & \text{if } 533K < T \le 1200K \\ 3.907\times10^{1} - 2.619\times10^{-2}T, & \text{if } 1200K < T \le 1311K \\ -2.305\times10^{1} + 3.366\times10^{-2}T, & \text{if } T > 1311K \end{cases} \tag{18}$$

FEM analysis is performed exploiting axisymmetrical geometry and a single strip is considered for simulations (Gür and Tekkaya, 1996). This assumption is employed since the passage of the moving workpiece through the heating and cooling rings promotes a localized phenomenon in this single strip while adjacent material, above and below this strip, is at lower temperatures.

At first, a numerical simulation is carried out in order to illustrate the potentiality of the proposed procedure to capture the general thermomechanical behaviour during quenching process. With this aim, PI hardening of a steel cylinder, 45 mm diameter and 180 mm length, subjected to an induced layer thickness e_{PI} = 3.5mm is considered. 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 (Camarão, 1998, Melander, 1985a). After that, the specimen is subjected to air-cooling until a time instant of 60s is reached. Figure (1) shows a mesh with 488 nodes and 842 elements employed in numerical simulations after a convergence analysis. The segment *OM* is at the cylinder centre axis while *LK* is at the cylinder surface. Null axial displacement condition is imposed in *OK* and *ML* in order to consider the restriction associated with adjacent regions of the heated region, which are at lower temperatures. Moreover, longitudinal heat conduction is neglected and thermal boundary conditions impose convection condition in *KL* while other faces have adiabatic conditions. Figure (1) also establishes a comparison between experimental results obtained by Camarão (1998) and those from numerical simulations obtained with the proposed model. Notice that results of volumetric fraction of martensite distribution are in close agreement (Silva *et al.*, 2004, Pacheco *et al.*, 2001a-b).

The forthcoming analysis considers the effect of local perturbations in the variables distribution during PI hardening, introducing a semi-circular notch in a long cylindrical steel bar. The cylinder has a notch with radius $r^* = 1$ mm and a thickness of induced layer, $e_{PI} = 5$ mm. Figure (2) shows a mesh for $r^* = 1$mm with 503 nodes and 904 elements, which is chosen after a convergence analysis. Similar symmetry and boundary conditions of the previous example are considered.

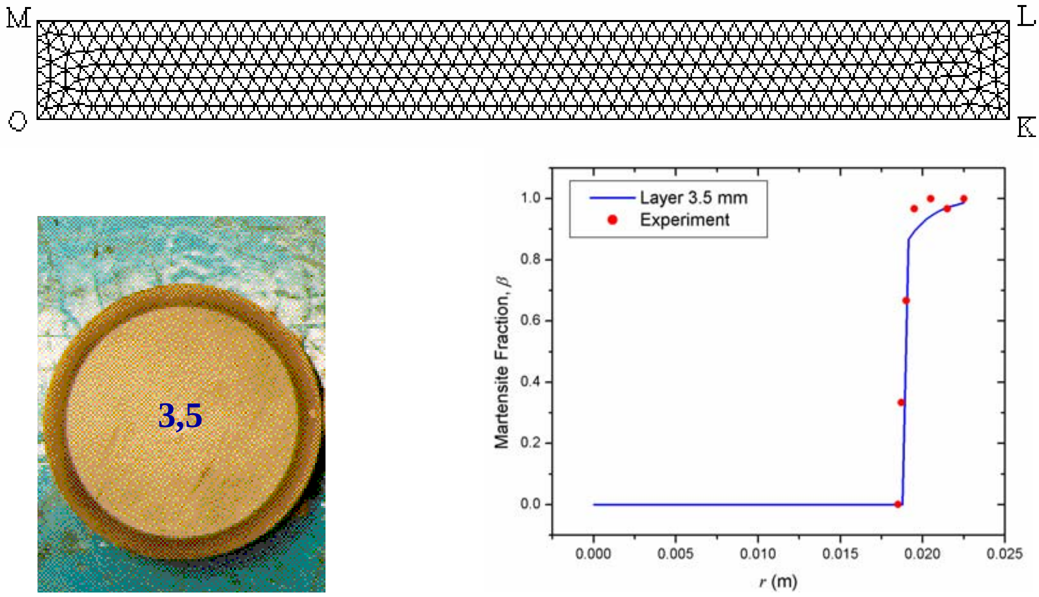

Figure 1. Comparison between numerical and experimental results. (a) Cylinder strip mesh. (b) Cross-sections of quenched bar submitted to a Nital etch 2%. (c) Volumetric fraction of martensite distribution for $e_{PI} = 3.5$ mm (Silva *et al.*, 2004, Pacheco *et al.*, 2001a-b, Camarão, 1998).

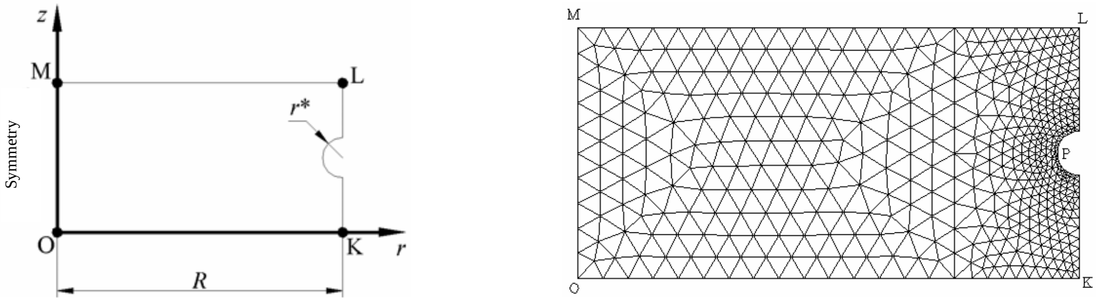

Figure 2. Cylinder strip with stress concentrator.

Residual stresses generated by quenching process is now focused on, comparing results predicted by two different models: *complete* (thermo-elastoplastic model with austenite-martensite phase transformation) and *without phase transformation* (thermo-elastoplastic model without phase transformation). Figure (3) presents results predicted by both models analysing von Mises stresses. Notice that the complete model has a larger critical region. Moreover, the model neglecting phase transformation underestimates results when compared to the complete model. This difference is about 7.5% for maximum von Mises stresses.

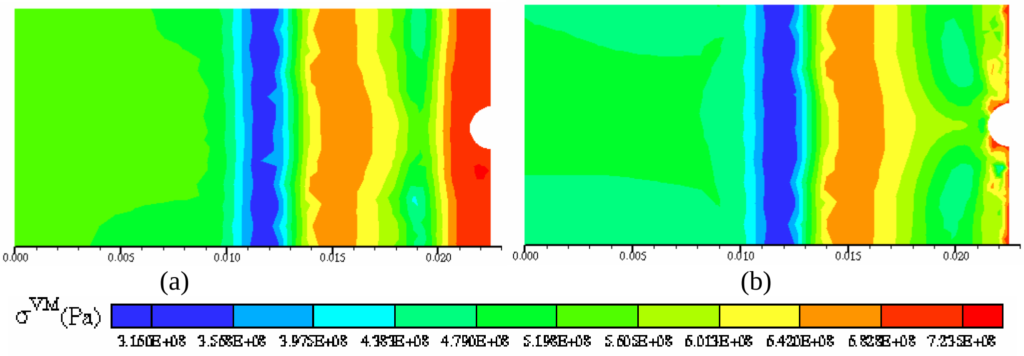

Figure 3. von Mises residual stresses. (a) *Complete* model; (b) Model *without phase transformation*.

Figure (4) presents a comparison between the results predicted by both models, taking data through the periphery of the notch. Notice that the complete model predicts compressive values in the entire notch surface, except at the edges where small tensile values are observed. On the other hand, the model without phase transformation predicts tensile stresses in some regions of the notch surface. This can be an important data for assessing the structural integrity of a mechanical component subjected to fatigue loadings. Since fatigue cracks usually initiate at the surface and propagate in the presence of tensile stress fields, tensile residual stresses at the surface can be especially critical.

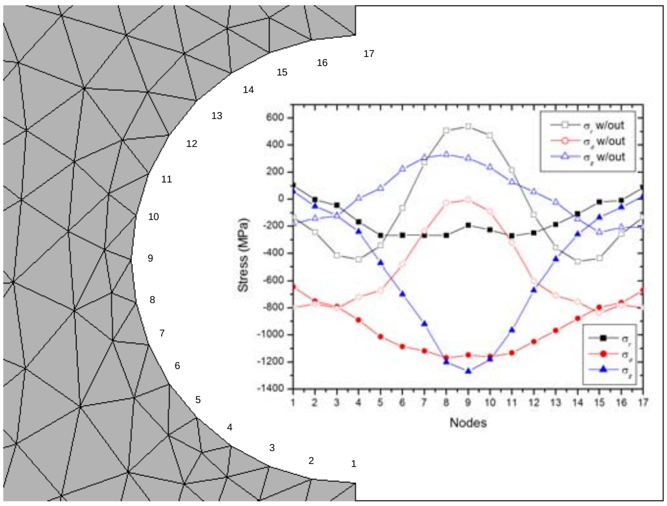

Figure 4. Residual stresses through the periphery of the notch for both models.

At this point, it is analysed data through the radius of the cylinder. Figure (5) presents a comparison between the results predicted by both models, showing that the notch introduces different perturbation in both models. Notice that far from the notch, where phase transformation does not occur, results predicted by both models are similar. Meanwhile, at the region between node 18 and the cylinder surface, the inclusion of phase transformation causes great discrepancies in the response of both models. Again, an important difference that should be pointed out is the variation of the sign of the stress components.

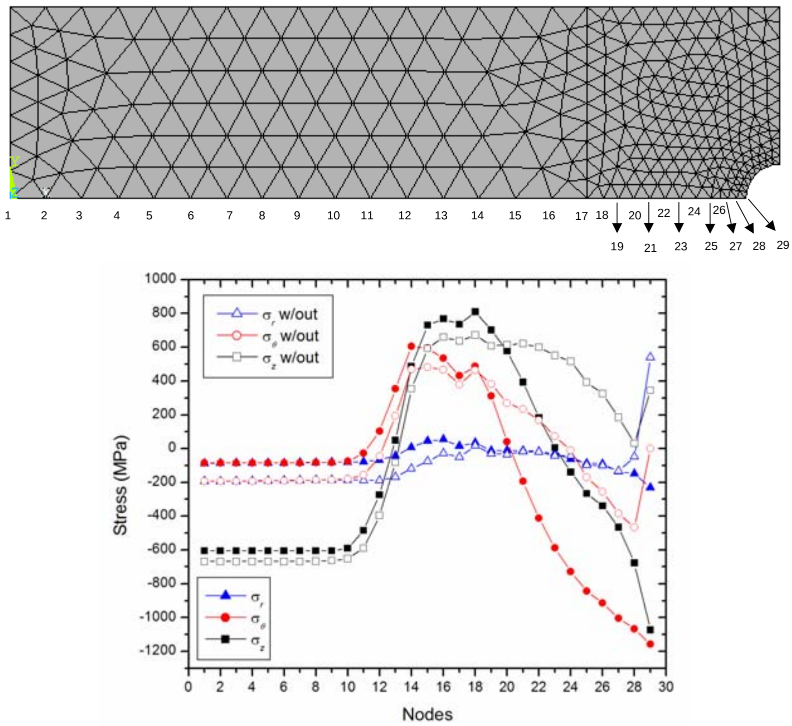

Figure 5. Residual stresses through the radius of the cylinder for both models.

5. Conclusions

This article presents a comparison between two different models employed to describe quenching process. The first one is a thermo-elastoplastic model that includes austenite-martensite phase transformation employing the constitutive model proposed by Pacheco *et al.* (2001a) and Silva *et al.* (2004). The second one is a thermo-elastoplastic model that neglects phase transformation. The finite element method is employed for spatial discretization. A numerical procedure is developed based on operator split technique associated with an iterative numerical scheme in order to deal with nonlinearities of the formulation. Progressive induction hardening of a steel cylindrical body with a semi-circular notch is considered. In general, it is possible to conclude that the model neglecting phase transformation underestimate values of residual stresses when compared to results predicted by the model that includes phase transformation. Moreover, differences related to the sign of the residual stresses may be expected between both models. These conclusions points to the necessity of including phase transformations during the prediction of residual stresses generated by the quenching process.

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