A NUMERICAL-EXPERIMENTAL METHODOLOGY TO CHARACTERIZE THERMOPLASTICS SUBJECT TO LARGE STRAIN USING A VARIATIONAL ELASTOPLASTIC MODEL

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Abstract. *Heterogeneous strain fields due to necking occurs on nonlinear elastoplastic materials, like thermoplastics, when submitted to finite strains. The prediction of this phenomenon with an adequate constitutive model requires a non-trivial numerical-experimental procedure since the resulting force data obtained from a tensile testing is not sufficient to assure the kinematics aspects of the necking. In order to determine the constitutive response of an elastoplastic material, this paper presents a numerical-experimental methodology combining numerical methods and experimental data obtained from mechanical testing with optical measurements. A variational constitutive model for nonlinear elastoplastic materials is implemented on a finite element method code, where the experimental conditions observed in mechanical testing are reproduced in a numerical simulation. The force history, obtained from the load cell, and the displacement field of the necking region, obtained from the optical measurement system, are used in a parameter identification procedure of the variational material model. A suitable objective function is proposed in order to take into account the necking phenomenon. The proposed methodology is applied on polyvinyl chloride (PVC) specimens, where tensile tests are performed. This methodology allows to evaluate the capability of the material model to reproduce simultaneously the results of force and necking displacement field.*

Keywords: *non-linear materials, optical measurement, variational model*

1 INTRODUCTION

Thermoplastic materials are present in an enormous variety of components produced by the industry. The material attractiveness reside on its low cost for complex geometries production, combined with large scale processing and low temperature/pressure of manufacture. Various properties from thermoplastic materials can be altered in its production and processing, enabling diverse engineering applications (Larson, 2015). However, the use of thermoplastics in structural applications, where it is submitted to high mechanical stress, is still restrict due to the highly nonlinear behavior, even at low temperature and strain.

The previous knowledge of the mechanical response is important to choose a suitable material model for a structural analysis of a component submitted to finite strains. Also, constitutive models sufficiently accurate and simple (regarding the number of material parameters) are needed to represent the observed mechanical behavior.

Thermoplastics submitted to large strains, in an uniaxial testing, present plasticity and a particular necking behavior that propagates to the entire specimen. The necking behavior in thermoplastics is a result of an instability phenomenon highly dependent of the specimen geometry modification during the mechanical test. The necking development governs the nominal stress response masking the real stress-strain behavior of the material (Frank and Brockman, 2001).

Numerical-experimental methodologies have been proposed to study the necking behavior and its importance into the mechanical behavior of thermoplastic materials (Ye et al, 2015; Vassoler and Fancello, 2011). In (Vassoler and Fancello, 2011), it is proposed a methodology to obtain the material parameters of a multilinear elastoplastic model in order to numerically characterize the mechanical behavior of a PVC specimen. Despite the simplicity of this model the authors achieved good results of the necking kinematics and reaction force in the specimen, which was measured by a load cell. Also, it is shown that the kinematic behavior of the necking is an important information to characterize thermoplastics that present significative necking. In order to perform this study, the authors used data from an uniaxial testing of a notched specimen, with optical measurement of the necking, in order to obtain suitable experimental data to be applied on an identification parameter procedure.

In this paper the numerical-experimental methodology proposed in (Vassoler and Fancello, 2011) is extend in order to use a variational visco-elastoplastic model proposed by (Fancello et al, 2008), which is capable to represent a continuous nonlinear response such as observed in thermoplastic materials. This hiperelastic-like model allows to choose the most appropriated elastic and dissipative energies found in literature to represent the desired mechanical response, improving the numerical characterization.

2 VARIATIONAL MODEL

The variational constitutive model proposed in (Fancello et al, 2008) is based into the assumption of the existence of a state variables set $\xi = \{\mathbf{F}, \mathbf{F}^i, \mathbf{Q}\}$ necessary to define the thermodynamical state of a material point, where $\mathbf{F}$ is an external state variable that represents the total deformation gradient tensor, $\mathbf{F}^p$ is an internal state variable that represent the plastic deformation gradient tensor, and $\mathbf{Q}$ is a subset of (scalar, vector, tensor) internal state variables that may represent other internal mechanisms of interest. Then, the free energy W can be written as a function of the set ξ:

$$W = W(\mathbf{F}, \mathbf{F}^p, \mathbf{Q}) \tag{1}$$

Irreversible mechanisms, like plasticity, are take into account assuming the existence of a dissipative pseudo-potential $\psi(\dot{\mathbf{Q}}, \dot{\mathbf{F}}^p)$, convex and null at the origin.

With these assumptions, an incremental potential, consistent with the evolution of the internal state variables, is written as (Fancello et al, 2008):

$$\Psi(\mathbf{F}_{n+1}; \xi_n) = \min_{\mathbf{F}^p_{n+1}, \eta_{n+1}} (W_{n+1} - W_n + \Delta t\, \psi(\mathring{\mathbf{F}}^p, \mathring{\mathbf{Q}})) \tag{2}$$

where $\mathring{\mathbf{F}}^p$ and $\mathring{\mathbf{Q}}$ are rate approximations of $\dot{\mathbf{F}}^p$ and $\dot{\mathbf{Q}}$.

This expression provides a potential for the First Piola-Kirchhoff stress tensor, analogously to hyperelastic materials, by:

$$\mathbf{P}_{n+1} = \frac{\partial \Psi(\mathbf{F}_{n+1}; \xi_n)}{\partial \mathbf{F}_{n+1}}, \tag{3}$$

A rheological mechanical model that represent the elastoplasticity response of this proposal is shown in Fig. 1.

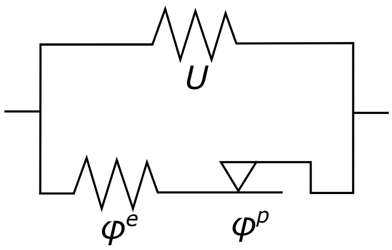

Figure 1: Representative mechanical model

In order to apply the variational framework for plasticity models is convenient to split the free energy potential as:

$$W(\mathbf{F}, \mathbf{F}^p, \mathbf{Q}) = U(J) + \varphi^e(\hat{\mathbf{C}}^e) + \varphi^p(\hat{\mathbf{C}}^p, \mathbf{Q}) \tag{4}$$

where J is the jacobian of $\mathbf{F}$, tensors $\hat{\mathbf{C}}^e$ and $\hat{\mathbf{C}}^p$ are, respectively, the elastic and permanent isochoric right Cauchy-Green tensors, that can be obtained from the elastic $\mathbf{F}^e$ and plastic $\mathbf{F}^p$ terms of the multiplicative decomposition of the isochoric gradient of deformation $\hat{\mathbf{F}}$:

$$\hat{\mathbf{F}} = J^{-\frac{1}{3}}\mathbf{F} \qquad \hat{\mathbf{F}} = \hat{\mathbf{F}}^e \hat{\mathbf{F}}^p$$

The evolution of the internal variable $\hat{\mathbf{F}}^p$ is related to the plastic stretching tensor $\mathbf{D}^p$ conveniently parameterized as (Fancello et al, 2008):

$$\mathbf{D}^p = \dot{q} \sum_{i=1}^{3} q_i \mathbf{M}^p_i \tag{5}$$

where $\dot{q}$ accounts for the amplitude of $\mathbf{D}^p$ while q_i and $\mathbf{M}_i^p$ for its direction. Using the exponential mapping, the update value of $\mathbf{F}^p$ is approximated by:

$$\mathbf{F}_{n+1}^p = \exp[\Delta t \mathbf{D}^p]\mathbf{F}_n^p = \exp[\Delta q \sum_{i=1}^{3} q_i \mathbf{M}_i^p]\mathbf{F}_n^p \tag{6}$$

The free energy associated to hardening/softening effects is simplified to be isotropic and consequently depending on the accumulated plastic amplitude q, such as:

$$\varphi^p(\hat{\mathbf{C}}^p, \mathbf{Q}) = \varphi^p(q) \tag{7}$$

$$q(t) = \int_0^t \dot{q}\mathrm{d}t = q_n + \Delta q \tag{8}$$

The dissipative potential ψ^p is defined to be function of $\dot{q}$, with penalization for negative values:

$$\psi^p(\mathbf{D}^p) = \psi^p(\dot{q}) = \psi^p\left(\frac{\Delta q}{\Delta t}\right) \tag{9}$$

where $\dot{q} \geq 0$ and $\psi^p(\dot{q})$ can be defined by different expressions.

The minimizing variables $\mathbf{Q}$ and $\mathbf{F}^p$ are replaced by Δq, q_i and $\mathbf{M}_i^p$, and the incremental potential is now represented by (Fancello et al, 2008):

$$\Psi = \Delta U(J_{n+1}) + \min_{\Delta q, q_i, \mathbf{M}_i^p}\left\{\Delta\varphi^e(\hat{\mathbf{C}}_{n+1}^e) + \Delta\varphi^p(\Delta q) + \Delta t \psi^*\left(\frac{\Delta q}{\Delta t}\right)\right\} \tag{10}$$

where

$$\Delta\varphi^e(\hat{\mathbf{C}}_{n+1}^e) = \varphi^e(\hat{\mathbf{C}}_{n+1}^e) - \varphi^e(\hat{\mathbf{C}}_n^e)$$
$$\Delta\varphi^p(\Delta q) = \varphi^p(q_n + \Delta q) - \varphi^p(q_n)$$

The first order optimality condition of the incremental potential Eq. (10) with respect to $\mathbf{M}_i^p$ results in $\mathbf{E}_i^e = \mathbf{M}_i^p$. The minimization with respect to the other internal variables Δq, q_i results in six nonlinear equations (Fancello et al, 2008):

$$\begin{aligned}
-\tfrac{\partial\varphi^e}{\partial\varepsilon_1^e}\Delta q + \lambda + 2\beta q_1 &= 0 \\
-\tfrac{\partial\varphi^e}{\partial\varepsilon_2^e}\Delta q + \lambda + 2\beta q_2 &= 0 \\
-\tfrac{\partial\varphi^e}{\partial\varepsilon_3^e}\Delta q + \lambda + 2\beta q_3 &= 0 \\
-\left(\tfrac{\partial\varphi^e}{\partial\varepsilon_1^e}q_1 + \tfrac{\partial\varphi^e}{\partial\varepsilon_2^e}q_2 + \tfrac{\partial\varphi^e}{\partial\varepsilon_3^e}q_3\right) + \tfrac{\partial\varphi^p}{\partial\Delta q} + \tfrac{\partial\psi^p}{\partial\dot{q}} &= 0 \\
q_1 + q_2 + q_3 &= 0 \\
q_1^2 + q_2^2 + q_3^2 &= \tfrac{3}{2}
\end{aligned} \tag{11}$$

where λ and β are Lagrange multipliers. The nonlinear Eq. (11) are solved by the Newton method and the first Piola-Kirchhoff stress tensor is calculated by Eq. (3). Detailed information about this model are found in (Fancello et al, 2008).

2.1 Material Models

Different material models can be used to represent the elastic and plastic mechanical behavior on this mathematical framework. This model is capable to represent a simple bilinear behavior of elastoplastic models, or even a highly nonlinear visco-elastoplastic response depending of the choice of the potentials. In this first approach it is chosen as elastic function φ^e the well-known hyperelastic Hencky potential and as plastic function φ^p a hardening law proposed in (Fancello et al, 2008):

$$\varphi^e = \sum_{i=1}^{3} \mu \varepsilon_i^{e2} \tag{12}$$

$$\varphi^p = \Sigma_0 q + \frac{1}{2} H q^2 + \mu^p \left(q + \frac{1}{\alpha^p} exp(-\alpha^p q) \right) + \frac{\mu^p_{pot}}{\alpha^p_{pot} + 1} q^{\alpha^p_{pot}+1} \tag{13}$$

where the state variable q is a scalar that represents plastic deformation accumulation and ε_i are the principal logarithmic strains of the deviatoric logarithmic strain $\varepsilon = 0.5 \ln \hat{\mathbf{C}}^e$. The vector of material parameters corresponding to this choice is given by:

$$\mathbf{p} = \; [\mu \quad \Sigma_0 \quad H \quad \mu^p \quad \alpha^p \quad \mu^p_{pot} \quad \alpha^p_{pot}] \tag{14}$$

Since it is the first study where this variational model is applied in such methodology, the choice of the potentials was based on the reduced number of material parameters. Should be noted that the resulting variational model can not represent viscosity phenomena, but it can represent elastoplaticity with a nonlinear hardening law, capable to accurately simulate the mechanical hardening observed in thermoplastics with significative necking.

3 METHODOLOGY

In order to obtain the material parameters of a model an inverse problem must be solve. Here it is used the same methodology and experimental data of (Vassoler and Fancello, 2011). The methodology is based on a Finite Element Method Updating procedure (FEMU) were the parameters are acquired from a updating strategy using numerical data obtained from a finite element (FEM) software. In this particular case, displacement data from the necking region are used into this strategy.

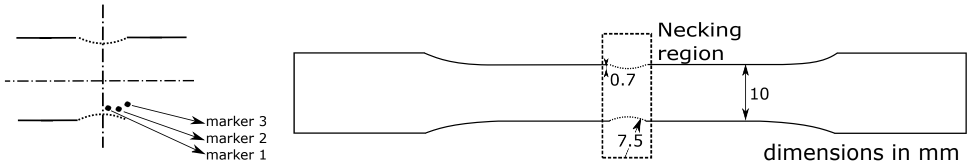

Figure 2: Markers positions and specimen geometry

The experimental data was obtained of a polyvinyl chloride (PVC) specimens submitted to tensile testing (see Vassoler and Fancello (2011)). Monotonic and cyclic uniaxial tensile testing are performed. From the monotonic testing it was taken the force reaction history and the transversal displacement of the markers 1, 2 and 3 (see Fig. 2). The cyclic tensile test, which is a sequence of loading/unloading/loading, supply only force data for this methodology in order to provide information about permanent strains, when submitted to large deformation.

Parameter identification procedure is performed minimizing a objective function Π, that take into account the reaction force, measured by a load cell, and transversal displacements of points on the surface of the necking region, measured by an optical measurement system (see Fig. 2):

$$\Pi(\mathbf{p}) \;=\; \sum_{j=1}^{n}\left(\frac{F_j^{FEM}(\mathbf{p})-F_j^{EXP}}{\max(\mathbf{F}^{EXP})}\right)^2 \;+\; \sum_{j=1}^{n}\left(\frac{u_j^{FEM}(\mathbf{p})-u_j^{EXP}}{\max(\mathbf{u}^{EXP})}\right)^2 \tag{15}$$

where $\mathbf{p}$ is a vector with the material parameters of the variational model, n is the number of points in the time-discretized data used to evaluate the objective function, $\mathbf{F}^{EXP}$ is the vector of reaction load measured by the load cell, $\mathbf{F}^{FEM}$ is the vector of reaction load computed by the FEM software, $\mathbf{u}^{EXP}$ is the vector with transversal displacements of points in the necking region, measured by the optical system (time-discretized) and $\mathbf{u}^{FEM}$ is the vector with the transversal displacements of the same points, computed by the FEM software. The force and displacement vectors are appropriately constructed (concatenated) to include monotonic and cyclic data. Should be noted that the original proposal (Vassoler and Fancello, 2011) used weighting parameters in the objective function to make more significant force or displacements, depending of the interest. Here, no weighting schemes have been used.

The minimization of Π respect to the parameters $\mathbf{p}$ gives the optimum set of material parameters that minimize the difference between the numerical and experimental data, taking into account the displacement of the necking region. The parameter identification procedure, based on a FEMU strategy, is schematically presented in Fig. 3.

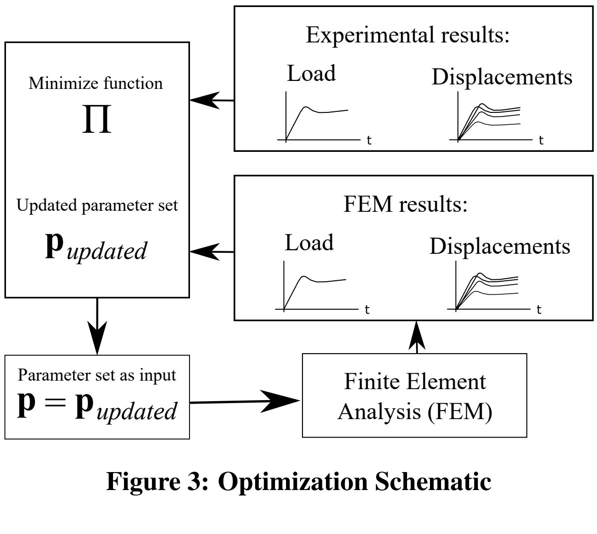

Figure 3: Optimization Schematic

In order to obtain the numerical results $\mathbf{F}^{FEM}$ and $\mathbf{u}^{FEM}$, the variational constitutive model and a tangent stiffness matrix were implemented on the USERMAT subroutine of the finite element software ANSYS. The tangent stiffness matrix uses a numerical approximation by forward differences (Sun et al, 2008) of Green-Naghdi stress rate, following the work of (Waas et al, 2012).

Table 1: Optimized parameters set

Elastic		Plastic					
μ	870	Σ_0	49.1	μ^p	5.21	μ^p_{pot}	149.7
		H	-39.6	α^p	102	α^p_{pot}	2.22

4 RESULTS

The force and transversal displacements results of the monotonic test are shown in the Figure 4 and the force results of the cyclic test in the Figure 5. The material parameters obtained by the optimization procedure are presented in Table 1 and the resulting real stress-strain curve is presented on Fig. 6.

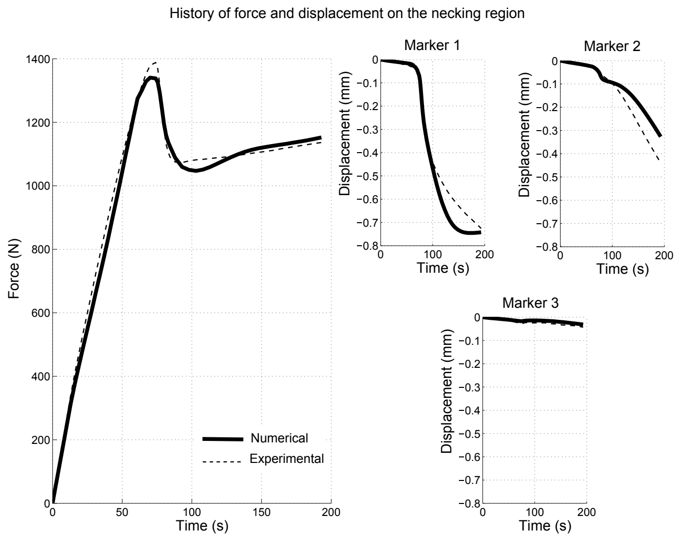

Figure 4: Monotonic test.

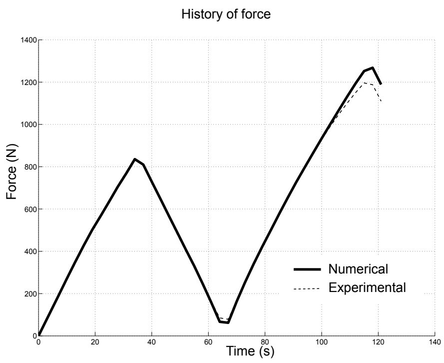

Figure 5: Cyclic test.

5 CONCLUSIONS

The proposal to implement the variational constitutive model into a numerical-experimental methodology, in order to improve the numerical representation, was accomplished. The variational model was implemented into a commercial FEM software and shown satisfactory results

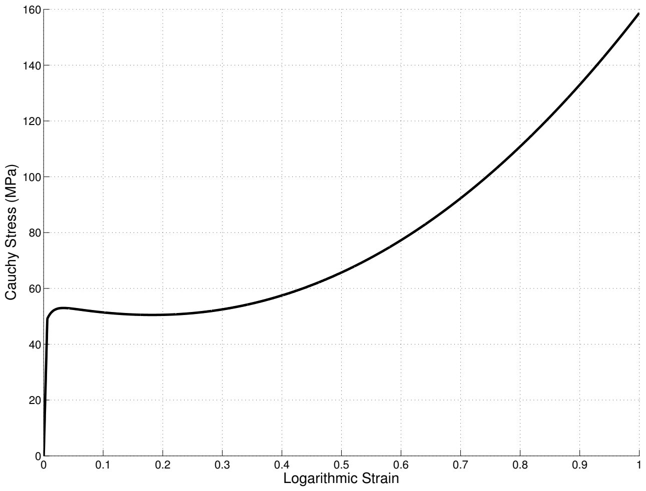

Figure 6: Stress versus strain graph from Table 1 parameters set

with less material parameters than the original material model (multilinear elastoplastic model). The resulting mechanical behaviour observed in Fig. 6 is very similar with the expected response of a ductile thermoplastic. In this first approach, only an elastoplastic nonlinear part had an active role in this study due to the elastic and plastic potentials choice. No viscous effects was included despite the fact that the variational model easily allows their use. Also, here was not studied different relationships between the force and displacement data into the objective function, such as that performed in the original work by using weighting parameters.

The use of the complete capability of the implemented model (viscous effects), associated to a rigorous study of the contribution of the force and displacement on the objective function, could significantly improve the numerical results.

ACKNOWLEDGEMENTS

The authors thanks financial support from CAPES, CNPq and FAPERGS in this work realization.

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