STUDY OF MECHANICAL BEHAVIOR FOR A BIOPOLYMER: EXPERIMENTAL TESTS AND NUMERICAL SIMULATIONS

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Abstract. *Nowadays, new materials have been developed to be used on human prosthesis. Due to many advantages, biopolymer is a very interesting alternative. However, the design of biopolymer prosthesis requires knowing how to predict the mechanical behavior of this material. This work consists on a study of material models (constitutive equations) in order to simulate the mechanical behavior of biopolymer obtained from the castor oil polyurethane (Ricinus communis). For the application of models, it was necessary to determine the material properties, as well as to understand the behavior of the biopolymer. Thus, specimens were manufactured following the standards published by American Society for Testing and Materials. After, tensile experimental tests were carried out for monotonic and cyclic loads, investigating the creep phenomenon. The parameters of von Mises, Drucker-Prager and viscoelastic models were obtained from the experimental results and input at the program Abaqus^{TM}. Finite element analyses, for monotonic loads, were performed. Computational results were compared to the experimental results and the errors between numerical and experimental tests are very low.*

Keywords*: biopolymer; material model; experimental tests; finite element analysis*

1. INTRODUCTION

During the last century, the humanity has improved the quality of life conditions, so, the life expectative has increased. This situation has occurred, mainly, due to technologic advances on different research areas (Etchebehere, 1998). For example, surgeries for bone reconstitution are more common, because the population is getting old (Wregge, 2000), and the bone implants must attend satisfactorily the functions executed by the part removed. Therefore, the structure implanted needs to support the loads on service and to minimize the problems with rejection. An alternative way to solve these requirements consists on to use biopolymers to manufacture the prosthesis like shown on work developed by Katti (2004). According to Ereno (2003), a biopolymer obtained from the castor oil polyurethane (*Ricinus communis*), developed by Chemistry Institute of São Carlos, is biocompatible and the possibility to rejection is very low. However, it is important to mention that this work will not discuss about aspects related to biological studies. In fact, the focus on the application of material models in order to simulate the mechanical behavior of the biopolymer obtained from the castor oil polyurethane (*Ricinus communis*).

Therefore, for the application of models, it was necessary to determine the material properties, as well as to understand the behavior of the biopolymer. Thus, specimens were manufactured following the standards published by American Society for Testing and Materials. After, tensile experimental tests were carried out for monotonic tests and in order to preliminary investigation the creep phenomenon; cyclic tests were performed, too. The parameters of material models were obtained from the experimental results and input at the program Abaqus^{TM}. Finite element analyses were performed and computational results were compared to the experimental results.

2. MATERIAL AND METHODS

2.1. Biopolymer

The biopolymer is synthetic polyurethane from a castor oil of *Ricinus communis*. The polyurethane is constituted by two components called pre-polymer 329L and poliol 471. In order to obtain the biopolymer, it is necessary to mix one portion of pre-polymer 329L to 0.7 portion of poliol 471 in mass. This process requires moisture control (40% of relative air humidity) and temperature control (nearly 20^{o}C). If the environment conditions are not controlled, the humidity is absorbed and reacted to the pre-polymer, releasing CO_2 and creating voids in the biopolymer.

2.2. Experimental Tests

The tensile tests followed the orientations of ASTM D638M – 96 (Type I), which describes specimen geometry like shown at Fig. 1a and the velocity of the test equal 5 mm/min (i.e. strain rate equal $1.67x10^{-3}s^{-1}$). However, after some experimental tests, the velocity of test was reduced to 0.8 mm/min (i.e. strain rate equal $2.67x10^{-4}s^{-1}$), not only for monotonic tensile tests, but also, for cyclic tensile tests (creep tests). It is important to mention that the results were obtained from extensometers in axial and transversal direction (Fig. 1b), as well as, unidirectional and biaxial strain gages for large strains - up to 15% (KYOWA, 2004a).

First of all, monotonic tensile tests were carried out by Universal Machine Test with displacement control. From the results (Fig. 2(a)), it was possible to calculate the Young modulus, Poisson's ratio, and yield and rupture stress for the biopolymer under tension load.

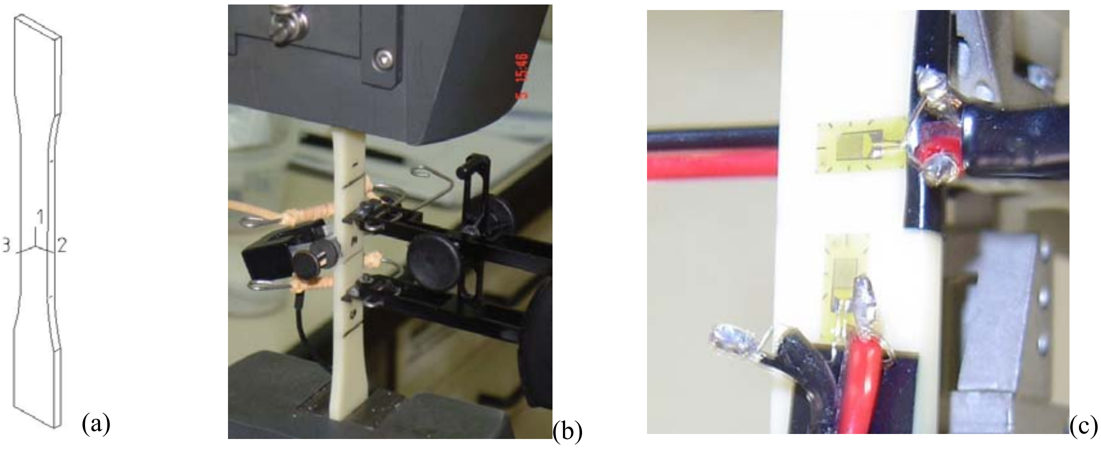


Figure 1. Tensile tests (ASTM D638): (a) specimen geometry; (b) displacement measures; (c) strain gage measures.

After that, the cyclic tests were carried out by cycles of loading, unloading and re-loading of the specimen in order to evaluate the biopolymer behavior in function of the time. Thus, the creep tests were executed by force control, using a Universal Machine Test. From the results, it was possible to analyze the curves load-displacement, stress-strain, as well as, the time when the material looses the response linearity, where it is calculated the elasticity and compliance modulus for creep. The cyclic tests (showed at Fig. 2(b)) follow 4 steps:

1) The velocity of the force applied is equal 37.5 N/s up to the specimen hits a specified value of force equal 250N (first landing);
2) For the first landing, the machine test is controlled in order to maintain the level of force (250N) for a time lag. Thus, the parameters associated to creep model can be determinate;
3) After the time lag, a ramp of force is applied using the same velocity (37.5 N/s) and a new landing is created for a force level equal 500N (second landing) during the same time lag in order to investigate the creep phenomenon;
4) The 3 steps before are carried out until a number of repetition specified. After that, a cycle with loading, unloading and re-loading is applied in order to investigate the recovery phenomenon during the unloading stage.

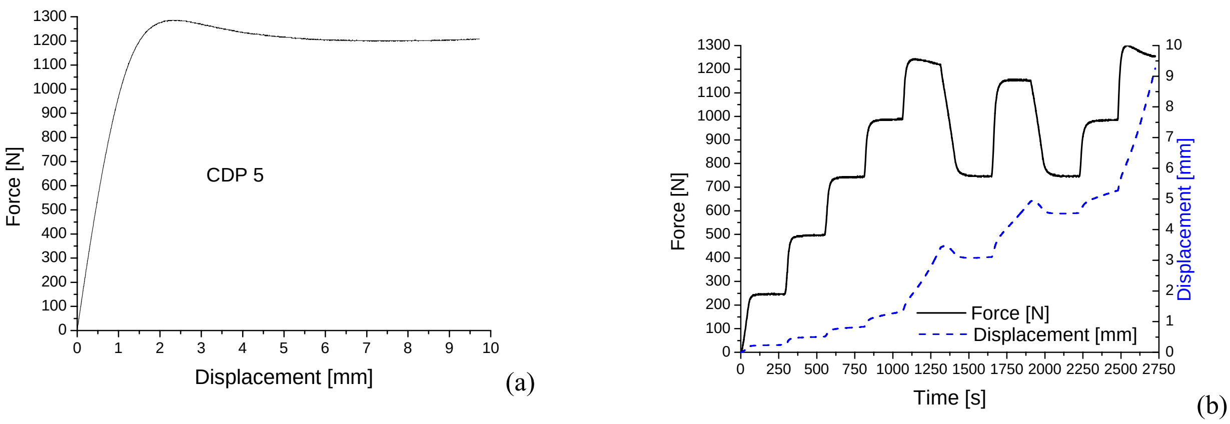


Figure 2. Experimental tests: (a) Monotonic Tests; (b) Cyclic Tests (procedure adopted)

2.3. Computational Simulations

The Finite Element Analysis (FEA) were performed, using software Abaqus^{TM}, in order to verify the limitation and potentials of material models to simulate the mechanical behavior under tension for the biopolymer. The dimensions are specified by the ASTM D638-96 (Type I), and according to the symmetry of the specimen for reducing the computational costs, it was used only 1/8 of the gage length (Fig. 3). Besides, due to the symmetry of the model and the necking phenomenon, it was applied boundary conditions like showed at Fig. 4(a) and 4(b). The model was meshed by 450 hexahedron elements called C3D8R with 8 nodes and 3 degree of freedoms for each one (displacement on x, y and z), the interpolation function is linear and the integration is reduced, the utility NLGEOM ON (geometric nonlinearity) was flagged (Hibbit et al, 2000).

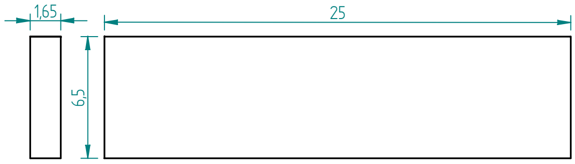


Figure 3. Geometry of model (1/8 of the gage length) – dimensions in mm.

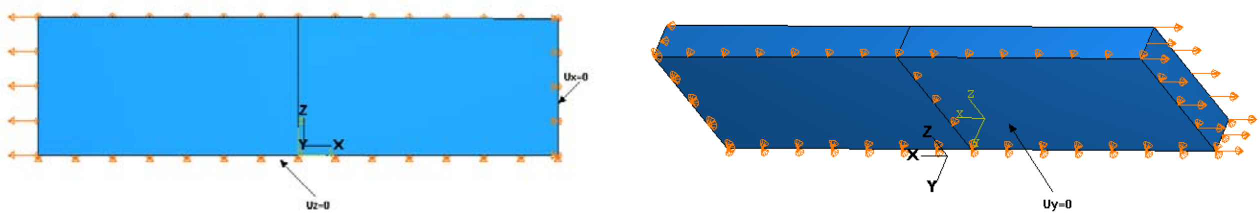


Figure 4. Boundary conditions applied for symmetry of the model and necking phenomenon

For the monotonic loading simulations, three different material models were used: 1) Elastoplastic model with von Mises' Criterion; 2) Elastoplastic model with Drucker-Prager's Criterion; 3) Viscoplastic model with von Mises' Criterion. Details about the formulations are described at Hibbitt et al (2002).

In order to input data for each model, it was used experimental curves like showed at Fig. 5. For example, Young modulus equal 1.47 GPa, and yield stress equal 30.73 MPa for von Mises' model. Otherwise, for Drucker-Prager's model, the yield stress was considered when the curve looses the linearity like showed at Fig. 5, i.e. at the final of proportionality limit (σ_v = 15.88 MPa at ε_v = 1.17%). Parameter values for Drucker-Prager's surface criterion are showed on Table 1. Besides, in order to avoid divergence numerical problems, the softening phenomenon observed in the experimental response was not considered for the elastoplastic analysis, only for viscoplastic analysis.

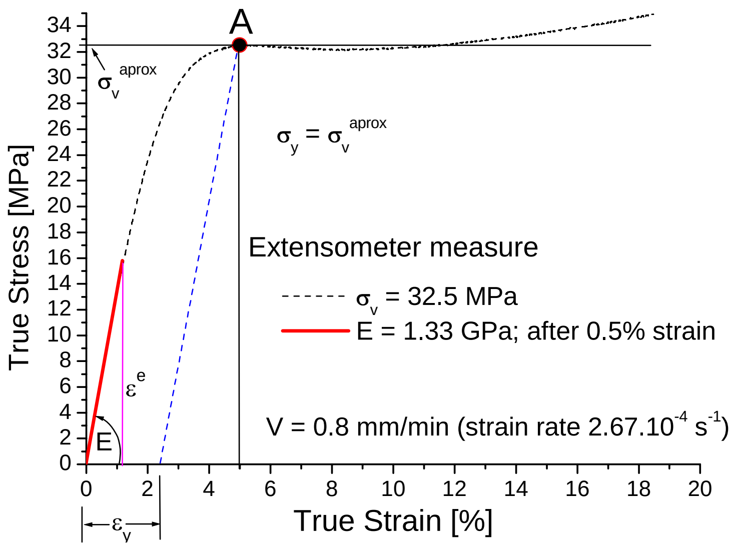


Figure 5. Curve true stress x true strain for the biopolymer (tensile test)

Table 1. Parameter values for Drucker-Prager's surface criterion

Parameters	Value
Fricton angle (β)	25.7°
Cohesion (d)	34.81 [MPa]
Dilatation angle (ψ) (Associative Law $\psi = \beta$)	25.7°

3. RESULTS AND DISCUSSIONS

3.1. Experimental Results of Monotonic Tests

In Figure 5, the necking phenomenon initializes at point A, when the specimen, initially, reduces its width, occurring the diffuse necking. After that, the specimen reduces its thickness and the stress state is not unidirectional, occurring the localized necking like described on Bridgman (1952), Ling (1996), Zhang et al (1999) and Zhang et al (2001). After point A, it is verified a softening behavior – stiffness reduction – up to 10% of strain, after this value, the material increase the stiffness due to hardening process. Then, the strain hits 18% without rupture of the specimen. This mechanical behavior is against of the hypothesis based on constant volume during yield process. In fact, during the yield process of polymer, the material volume changes with plastic strains (G'Sell et al, 2002). Thus, the equations used to calculate the stress and the strain of polymer material needs to consider the instantaneous volume. In order to calculate the material properties of the biopolymer, it was used extensometers or strain-gages biaxial measurements. For the strain gages, it was calculated the true stress σ_v by equation (1) and true strain ε_v by equation (2):

$$\sigma_v = \frac{F}{A} \tag{1}$$

$$\varepsilon_v = \int_{L_o}^{L_f} \frac{dL}{L} = \ln \frac{L_f}{L_o} \tag{2}$$

Where L_o is the initial gage length, L_f is the final gage length, F is the force obtained by the load cell, and A is the instantaneous transversal section area of the specimen obtained by:

$$A = w_i . t_i \tag{3}$$

$$w_i = w_0 . \left(1 - \frac{\varepsilon_v^{trans}}{100}\right) \tag{4}$$

$$t_i = t_0 . \left(1 - \frac{\varepsilon_v^{trans}}{100}\right) \tag{5}$$

Where w_o is the initial width, w_i is the instantaneous width obtained by the transversal strain ε_v^{trans}, which is measured by a strain gage. The instantaneous thickness t_i is obtained by the initial thickness t_o and the transversal strain, considering the material is transversally isotropy.

For the extensometer, it was calculated the true stress σ_v by equation (6):

$$\sigma_v = \frac{F}{A_{aprox}} \tag{6}$$

$$A_{aprox} = w_0 . \left(1 - \frac{\nu.\varepsilon_v^{long}}{100}\right) . t_0 \left(1 - \frac{\nu.\varepsilon_v^{long}}{100}\right) = w_i . t_i \tag{7}$$

Where ν is the Poisson's ratio equal 0.44 and longitudinal strain ε_v^{long} measured by extensometer.

Table 2. Material properties obtained from tensile tests for biopolymer
(E =Young modulus; σ_y^v = yield stress; ε_y^v = strain at yield stress)

Number	Extensometer Measurements			Strain gages Measurements		
	$\sigma_v = F/A_{aprox}$ (eq. 6)			$\sigma_v = F/A$ (eq. 1)		
	σ_y^v [MPa]	E [GPa]	ε_y^v [%]	σ_y^v [MPa]	E [GPa]	ε_y^v [%]
1	32.79	1.35	4.26	32.59	1.54	4.18
2	31.88	1.33	4.42	31.51	1.43	3.65
3	28.90	1.32	4.46	28.10	1.44	2.57
Average	31.19	1.33	4.38	30.73	1.47	3.47

The mediums values are:

$\sigma_y^v = 30{,}73$ MPa; $E_v = 1{,}47$ GPa; $\nu = 0{,}44$; $\varepsilon_y^v = 3{,}47\%$.

3.2. Experimental Results of Cyclic Tests

In Figure 7, it is verified that the material changes its mechanical behavior deeply after the viscoelastic regime. The Fig. 7 shows a result of creep test with three different regimes: (I) linear viscoelastic; (II) non-linear viscoelastic and (III) visco-elastoplastic. In general, it is important to note that the response of the material is very different when compared regime III to regime I and II, because it occurs a small increase of stress for a huge increase of strain. This observation is according to Williams (1973), because, polymers have linear viscoelastic regime up to 0.5% of strain.

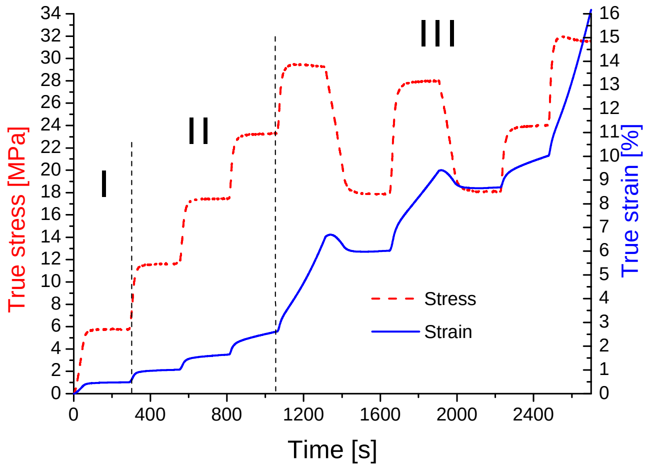


Figure 7. Results of creep tests: True stress x time and True strain x time

During the linear viscoelastic regime (I), the biopolymer does not creep, i.e. when the load hits the landing specified, the specimen maintains the strain level applied initially. In the non-linear viscoelastic regime (II), the biopolymer shows creep phenomenon, because, when the load hits the landing specified, the specimen increases the strain level. In the visco-elastoplastic regime (III), it is important to mention that the load applied was calculated by monotonic tests in order to create plastic strains. Thus, the load steps applied during regime (III) shows that the biopolymer can have recovery even on levels of permanent strain.

According to Fig. 8, there is a reduction of the stiffness when the specimen initializes the yield process at the landing V, because the biopolymer does not support the load applied. It is important to note that the same problem occurs at the landing VI and VII, because the specimen increases the strain, while the force is established on specified level. It is supposed that the deformation of the specimen is cause by a residual strain due to the level of the load at landing V and the reduction of the loading on the next cycles was not enough to reduce or to stop the yield flow process. However, the strain rate reduced when the load reduced too, at the landing VII. This observation is confirmed by the slope of the strain-time curve. Therefore, the compliance of the specimen increases drastically when the material hits higher levels of strain in tension.

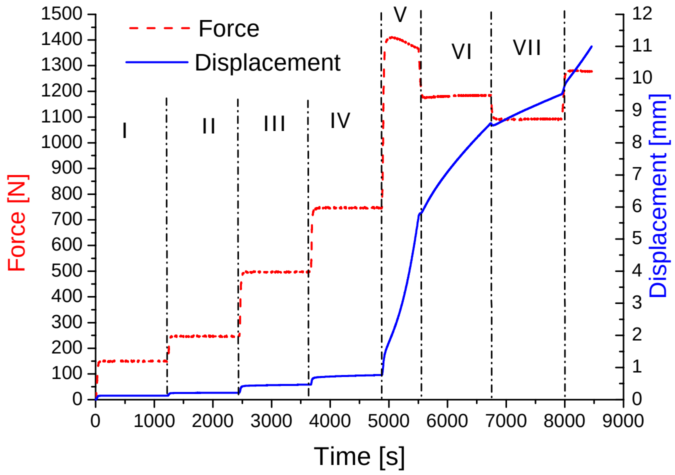


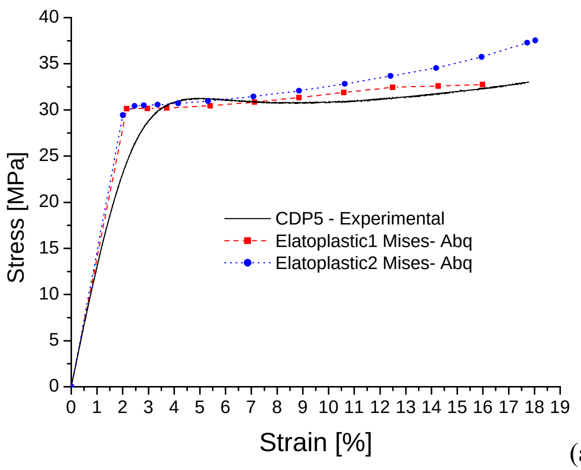
Figure 8. Results of creep tests: Force x time and Displacement x time

3.3. Numerical Results

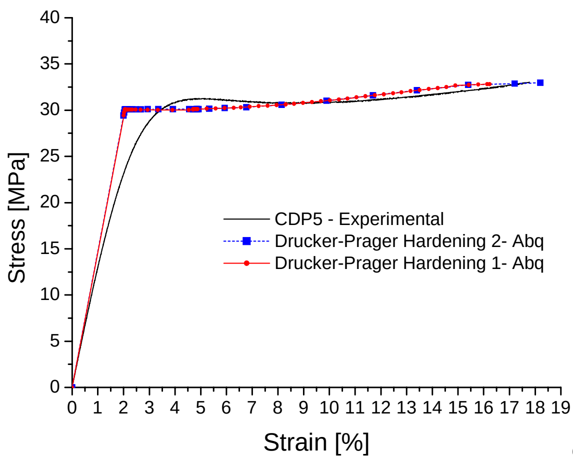
For the monotonic loading simulations, three different material models were used: 1) Elastoplastic model with von Mises' Criterion; 2) Elastoplastic model with Drucker-Prager's Criterion; 3) Viscoplastic model with von Mises' Criterion.

In Figure 9(a), there is a comparison between the numerical results obtained by elastoplastic model with von Mises' Criterion to experimental results. For the model 1 like showed by red curve in Fig. 9(a), the error for strain higher than 4% is nearly 3.3% between numerical and experimental result. However, this material model cannot simulate the biopolymer behavior with physical consistency, because the von Mises' Criterion considers that only deviatory stress tensor causes yield, and for polymer, the yield process is caused by deviatory and hydrostatic stress tensors. Thus, it was used an elastoplastic model with Drucker-Prager's Criterion.

In Fig. 9(b), there is a comparison between the numerical results obtained by elastoplastic model with Drucker-Prager's Criterion to experimental results. For these models, the error for strain higher than 4% is nearly 2.13% between numerical and experimental result. However, this material model cannot simulate the viscous effect. Therefore, it was evaluated a viscoplastic model with von Mises' Criterion.



(a)



(b)

Figure 9. Numerical and experimental results: (a) Elastoplastic model with von Mises' Criterion; (b) Elastoplastic model with Drucker-Prager's Criterion

In Figure 10, represented 1/8 of finite element model for tension test, show necking simulation behavior through Elastoplastic model with von Mises' Criterion. The number and type of finite elements applied with the option NL GEOM flagged produced good results. It is important to note the symmetry conditions showed on Fig. 4.

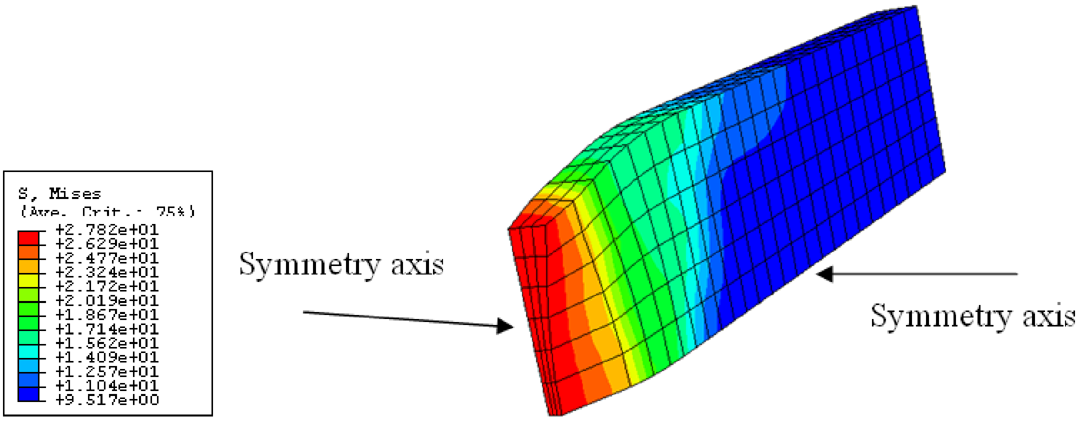


Figure 10. Necking phenomenon simulated by finite element model (1/8 of finite element model for tension)

In Figure 11 show the comparison among the theoretical and experimental curves, in which the best values of parameters of entrance of the model were the following ones: "A" equal to 0.18; "n" equal to 2.8; "m" equal to zero e "f" equal to 0.15205.

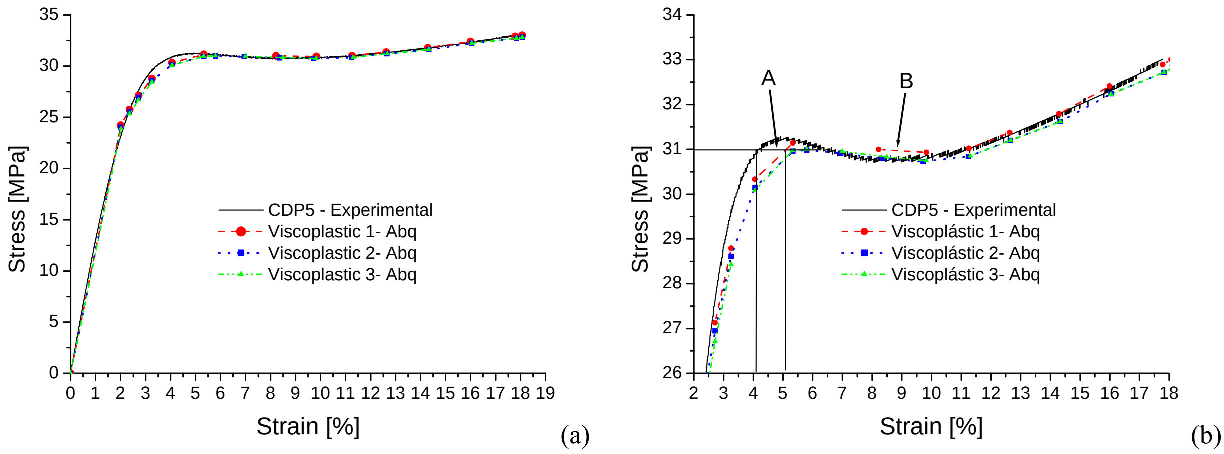


Figure 11. Numerical and experimental results for the viscoplastic model with von Mises' Criterion: (a) stress x strain curve; (b) detail of the viscoplastic region

In Fig.11, there is a comparison between the numerical results obtained by viscoplastic model with von Mises' Criterion to experimental results where the errors are very low. It is possible to verify that at point A (Fig. 11(b)), for the same level of stress, the strain experimental result is 4.184% and the numerical result is 5.049%, i.e., an error equal 20.7%. However, at the point B (Fig. 11(b)), for the same level of strain, the stress experimental result is 30.97 MPa and the numerical result is 30.97%, i.e., an error equal 0.61%. Thus, this model estimates a load level lower than the load level necessary to produce a yield process.

4. CONCLUSIONS AND FUTURE PERSPECTIVE

According to monotonic experimental results, it was possible to plot true stress x true strain curves using strain gages and extensometer measurements. Two different methods were applied and compared, because the volume of the polymer changes during the yield process. Based on the curves, it was determine the mechanical properties (Young modulus; yield stress; strain at yield stress) for the biopolymer, as well as, analyzed the mechanical behavior. In fact, the results showed by the two methods were very close, but, for simulations, it was used the results obtained from the strain gages. However, better results could be obtained if used image correlation technique to determine the deformation field.

According to cyclic experimental results, it is important to mention that this work is a preliminary study of the creep phenomenon. Therefore, the investigation focus on only the general mechanical behavior of the biopolymer. Thus, the creep curves show different regimes: (I) linear viscoelastic; (II) non-linear viscoelastic and (III) visco-elastoplastic. In general, it is important to note that the response of the material is very different when compared regime III to regime I and II, because it occurs a small increase of stress for a huge increase of strain.

According to the monotonic numerical results, the material models investigated show that the errors between numerical and experimental tests are very low. The comparison between the numerical results obtained by viscoplastic model with von Mises' Criterion to experimental results shows an error lower than 1% on prediction of stress. Thus, this model estimates a load level lower than the load level necessary to produce a yield process. Therefore, considering a structural design for an implant under tension, if this material model were applied, a positive margin of safety would be guaranteed.

For the future perspective, the cyclic tests for investigating the relaxation phenomenon can be carried out, as well as, an investigation of material models for simulating the biopolymer behavior under cyclic loads. It is important to mention, that the authors have developed research in these lines, and a technical paper will be submitted in the future.

5. ACKNOWLEDGEMENTS

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