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# NUMERICAL SIMULATION OF BIODEGRADABLE POLYMERS CONSIDERING VISCOPLASTIC BEHAVIOUR

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## ABSTRACT

A large range of biodegradable polymers have been used to produce implantable medical devices, such as suture fibres, fixation screws and soft tissue engineering devices. Apart from biological compatibility, these devices shall also be functional compatible and perform adequate mechanical temporary support during the healing process. However, the mechanical behaviour of biodegradable materials during its degradation, which is an important aspect of the design of these biodegradable devices, is still an unexplored subject. The viscoplastic constitutive models used in this work allow simulating the performance of biodegradable structures undergoing large deformations. Together they enable to simulate the monotonic tests of a biodegradable structure at different strain rates and it also enables to simulate hysteresis occurring in the unloading reloading cycles at different strain levels.

***Keywords:*** constitutive models, viscoplastic, biodegradable, materials.

## INTRODUCTION

A wide variety of material behaviors are described with a few different classes of constitutive equations. Mechanical properties of biodegradable plastics are commonly assessed within the scope of linearized elasticity, despite the clear evidence that they can undergo large strains before breaking. Due to the nonlinear nature of the stress vs. strain plot, the classical linear elastic model is clearly not valid for large strains simulation. Other plasticity or hyperelastic models are required to model those situations. Hence, given the nature of biodegradable polymers, classical models such as the neo-Hookean and Mooney-Rivlin models, for incompressible hyperelastic materials, were used to predict mechanical behavior until rupture of non-degraded PLA (Lunt, 1998; Garlotta, 2001). However, these methods neglect any changes in the properties of the material during degradation. Recent developments of hyperelastic constitutive models enable the modeling of biodegradable structures during degradation (Soares, 2010; Vieira , 2011) considering that the constitutive model parameters are changed according to hydrolytic damage. However, these methods neglect the time-dependent mechanical behavior. In a more recent study (Muliana, 2012) a non linear viscoelastic model was used to model the time-dependent performance of biodegradable structures. This method enables to model the relaxation behavior (or creep) during degradation, and is reasonably good to model moderate deformations.

The viscoplastic constitutive models used in this work, the Bergström-Boyce model (Bergström, 1998), allow simulating the performance of biodegradable structures undergoing large deformations. Together it enables to simulate the monotonic tests of a biodegradable structure at different strain rates and it also enables to simulate hysteresis occurring in the unloading reloading cycles at different strain levels.

## CONSTITUTIVE MODELLING

The experimental results presented in a previous work (Vieira, 2010) clearly demonstrated the non-linear and time-dependent behaviour that is exhibited by a biodegradable polymeric blend of polylactic acid (PLA) and poly caprolactone (PCL) in proportion 90:10. To address this observations a constitutive model used to simulate the large strain time-dependent behaviour of elastomers, developed by Bergström and Boyce (Bergström, 1998), was use in this work. In this constitutive model, the mechanical behaviour is decomposed into two parts: an equilibrium response, modelled by a hyperelastic constitutive model (network A), and a time-dependent deviation from equilibrium, defined by a viscoplastic constitutive model (network B). Network B is composed of an elastic element (also modelled by a hyperelastic constitutive model) in series with a time-dependent element which acts to relieve the strain of network A with time. According to the rheological representation of the constitutive model, presented in figure 1, the material is modelled as two polymer networks acting in parallel.

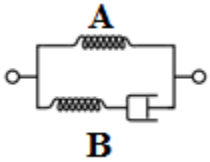


Fig.1 Rheological representation of Bergström-Boyce model

Finite deformation continuum mechanics requires the specification of reference and deformed configurations. Let X denotes the components of a Cartesian vector specifying a material point in the reference configuration. Then x(X, t) denotes the same material point in the deformed configuration, and represents the motion of this material point. The total deformation gradient is defined by:

$$F=\mathbf{F}_{ij}=\frac{\partial \mathbf{x}_i}{\partial \mathbf{X}_j}$$

Since deformation in network A is the same of network B, then $F=F_A=F_B$. The deformation gradient on network B can further be decomposed into an inelastic deformation followed by an elastic deformation ($F_B=F^e_BF^p_B$), where the inelastic deformation represents the configuration obtained by a complete virtual elastic unloading of network B to a stress free state.

The response of network A is given by the Arruda-Boyce model (Arruda, 1993), also known as eight chain model. The Arruda-Boyce eight-chain hyperelastic model is an extension of the neo-Hookean model that takes non-linear Langevin chain statistics into account when deriving the strain energy density function. The stress response of the eight-chain model is given as:

$$\sigma_A=\frac{\mu}{J\overline{\lambda^*}}.\frac{\mathcal{L}^{-1}(\overline{\lambda^*}/\lambda_L)}{\mathcal{L}^{-1}(1/\lambda_L)}\mathrm{dev}[\mathbf{B}^*]+\kappa(J-1)\mathbf{I}$$

where $\mu$ is the shear modulus, $\kappa$ the bulk modulus, and $\lambda_L$ is the limiting chain stretch. I is the second order identity tensor. $\overline{\lambda^*}$ is the applied chain stretch which can be calculated from:

$$\bar{\lambda}^* = \sqrt{\frac{\mathrm{tr}\mathbf{B}^*}{3}}$$

$\mathcal{L}^{-1}(x)$ is the inverse Langevin function, where $\mathcal{L}(x) = \coth(x) - 1/x$, is the Langevin function. $\mathbf{B}^* = J^{2/3}\mathbf{B} = J^{2/3}\mathbf{F}\mathbf{F}^T$ is the distortional left Cauchy-Green tensor and $\sigma_A$ is the Cauchy stress tensor a(also known as true stress tensor) acting in network A. The stress on network B is also given by the eigth-chain model:

$$\sigma_B = \frac{s\mu}{J_B^e \overline{\lambda_B^{e*}}} \cdot \frac{\mathcal{L}^{-1}(\overline{\lambda_B^{e*}}/\lambda_L)}{\mathcal{L}^{-1}(1/\lambda_L)} \mathrm{dev}[\mathbf{B}_B^{e*}] + \kappa(J_B^e - 1)\mathbf{I}$$

where $s$ is a dimensionless material parameters specifying the shear modulus of network B relative do network A, and $\overline{\lambda_B^{e*}}$ is the chain stretch in the elastic part of Network B. Using this representation the total Cauchy stress is given by: $\sigma = \sigma_A + \sigma_B$.

The velocity gradient on network B, $\mathbf{L}_B = \dot{\mathbf{F}}_B \mathbf{F}_B^{-1}$, and the deformation gradient on network B can be decomposed into elastic and viscoplastic components ($\mathbf{F}_B = \mathbf{F}^e_B \mathbf{F}^p_B$). Hence:

$$\mathbf{L}_B = \left[\frac{d}{dt}\left(\mathbf{F}_B^e \mathbf{F}_B^p\right)\right]\left(\mathbf{F}_B^e \mathbf{F}_B^p\right)^{-1} = \left[\dot{\mathbf{F}}_B^e \mathbf{F}_B^p + \mathbf{F}_B^e \dot{\mathbf{F}}_B^p\right]\left(\mathbf{F}_B^p\right)^{-1}(\mathbf{F}_B^e)^{-1} =$$
$$= \dot{\mathbf{F}}_B^e(\mathbf{F}_B^e)^{-1} + \mathbf{F}_B^e \dot{\mathbf{F}}_B^p\left(\mathbf{F}_B^p\right)^{-1}(\mathbf{F}_B^e)^{-1} = \mathbf{L}_B^e + \mathbf{F}_B^e \mathbf{L}_B^p (\mathbf{F}_B^e)^{-1} = \mathbf{L}_B^e + \widetilde{\mathbf{L}_B^p}$$

where the velocity gradient L can be decomposed into the sum of stretch rate and spin tensor D and W:

$$\mathbf{L}_B^p = \dot{\mathbf{F}}_B^p\left(\mathbf{F}_B^p\right)^{-1} = \mathbf{D}_B^p + \mathbf{W}_B^p$$
$$\widetilde{\mathbf{L}_B^p} = \widetilde{\mathbf{D}_B^p} + \widetilde{\mathbf{W}_B^p}$$

To make the unloading unique, $\widetilde{\mathbf{W}_B^p} \equiv 0$ is prescribed, according to (Bergström, 1998). The rate of viscoplastic deformation of network B is constitutively prescribed by:

$$\widetilde{\mathbf{L}_B^p} = \widetilde{\mathbf{D}_B^p} = \dot{\gamma}_B \mathbf{N}_B$$

where:

$$\mathbf{N}_B^v = \frac{\mathrm{dev}[\sigma_B]}{\tau} = \frac{\mathrm{dev}[\sigma_B]}{\|\mathrm{dev}[\sigma_B]\|_F}$$

give the direction of the driving stress state of the relaxed configuration and $\dot{\gamma}_B$ is an effective creep rate. $\tau = \|\mathrm{dev}[\sigma_B]\|_F$ is the effective stress driving the viscous flow. The time derivative of $\mathbf{F}_B^p$ can be derived as follows:

$$\widetilde{\mathbf{L}_B^p} = \mathbf{F}_B^e \dot{\mathbf{F}}_B^p\left(\mathbf{F}_B^p\right)^{-1}(\mathbf{F}_B^e)^{-1} = \dot{\gamma}_B \mathbf{N}_B^p$$

and hence:

$$\dot{F}_B^p = \dot{\gamma}_B (F_B^e)^{-1} \frac{\mathrm{dev}[\sigma_B]}{\|\mathrm{dev}[\sigma_B]\|_F} F_B^e F_B^p$$

The rate-equation for viscous flow is given by (Bergström, 1998):

$$\dot{\gamma}_B = \dot{\gamma}_0 \left(\overline{\lambda_B^p} - 1 + \xi\right)^C \left[R\left(\frac{\tau}{\tau_{base}} - \hat{\tau}_{cut}\right)\right]^m$$

where $\dot{\gamma}_0$ =1/s is a constant introduced to ensure dimensional consistency, *R(x) = (x + |x|)/2* is the ramp function, $\hat{\tau}_{cut}$ is a cut-off stress below which no flow will occur, $\tau_{base}$ represents the flow resistance, *m* is a stress exponential, $\xi$ is a strain adjustment factor, *C* is a strain exponential and:

$$\overline{\lambda_B^p} = \sqrt{\frac{\mathrm{tr}[F_B^p F_B^{pT}]}{3}}$$

## RESULTS

Suture fibres of PLA-PCL blend (90:10) of 0.4 mm and 50 mm long were monotonically tensile tested in an universal testing machine at displacement rates of 500 mm/min and 15 mm/min. In addition to these, cyclic tensile tests were carried out with cycles of loading and unloading until a minimum stress close to zero and, reloading up to different five strain levels. The experimental results clearly demonstrate the non linear time-dependent mechanical behaviour. In figures 2 and 3 one can see that the viscoplastic material model allowed a reasonable approximation of the experimental results. The inverse analyses to identify the parameters of the viscoplastic models used in this work were done using MCalibration software (Veryst Engineering). The model parameters identified by inverse parameterization are presented in table 1.

Table 1 List of the models parameters identified by inverse parameterization

| **Model parameters** | |
|---|---|
| $\mu$ **- Shear modulus of network A** | 353.794 |
| $\lambda_L$ **- Locking stretch** | 1.55181 |
| $\kappa$ **- Bulk modulus** | 73122.9 |
| ***s*** **- Relative stiffness of network B** | 1.03351 |
| $\xi$ **- Strain adjustment factor** | 0.125258 |
| ***C*** **- Strain exponential** | -0.554366 |
| $\tau_{base}$ **- Flow resistance** | 64.7435 |
| ***m*** **- Stress exponential** | 4.47534 |
| $\hat{\tau}_{cut}$ **- Normalized cut-off stress for flow** | 0.01 |

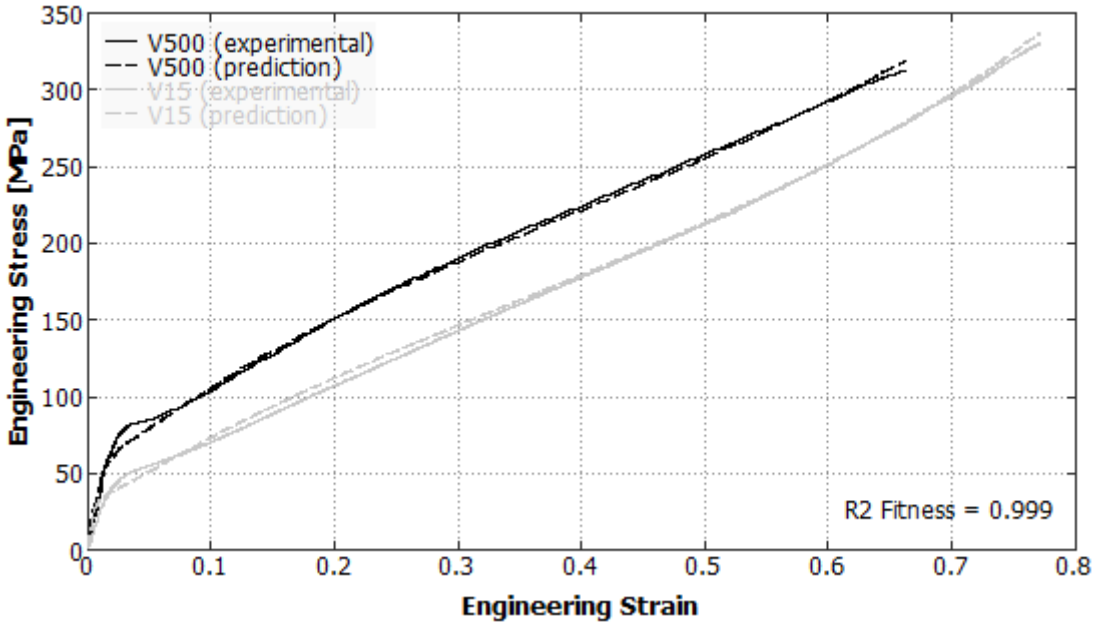


Fig.2 Experimental results of monotonic tensile test at two strain rates (500 and 15mm/min) of a biodegradable polymer (PLA-PCL), and prediction via viscoplastic Bergström-Boyce model

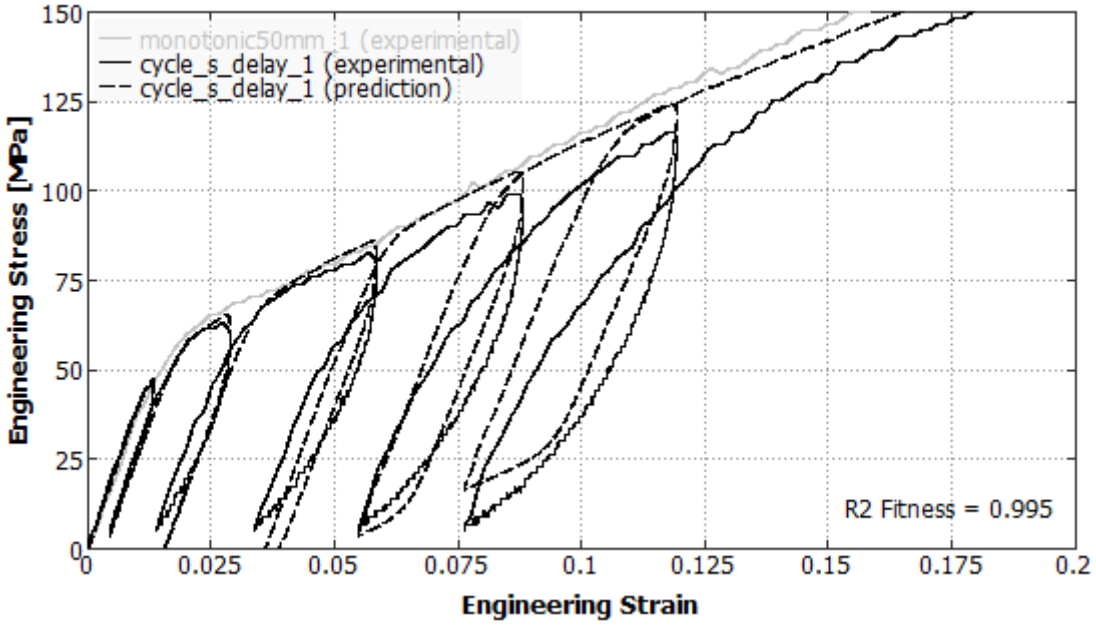


Fig.3 Experimental results of cyclic tensile test of a biodegradable polymer (PLA-PCL) and prediction via viscoplastic Bergström-Boyce model

## CONCLUSIONS

Biodegradable polymers are known by their non-linear and time-dependent mechanical behavior. Therefore, the constitutive viscoplastic models analyzed in this study were able to predict the viscoplastic behavior of PLA-PCL blend used. Although this approach was only evaluated for this particular blend, the authors believe that this can be extended to other

thermoplastic biodegradable materials above its glass transition temperature, since it was originally developed for engineering rubbers and other soft materials with both non-linear and time-dependent mechanical behavior. Although this model is much more complex than the hyperelastic models usually used to model the mechanical behavior of biodegradable polymer, it enables to simulate realistic loading cases usually similar to those in service. These in service loading cases comprise loading at various rates, cyclic loading or even relaxation and creep. Similarly to other methods of predicting the mechanical behavior evolution during hydrolytic degradation, the material parameters evolution according to hydrolytic damage will be the aim of future studies.

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