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Abstract

The objective of this work is to propose a dual finite deformation visco-hypoelasticity model and a numerical scheme for the analysis of polimeric materials. The proposed rate form of constitutive equation is formulated in terms of objective Green-Naghdi rate Kirchhoff stress tensor and Lagrangian logarithm (Hencky) strain tensor rate. The integration of the rate constitutive equation yields an integro-differential form of constitutive equation. The material is assumed to be isotropic and the kernel functions, associated with the shear and bulk compliance modulus, are represented in Prony series. The problem is formulated within a Total Lagrangian descripton. The Galerkin finite element method is used for numerical approach. Finally some problem cases are solved, and the proposed model, the robustness and performance of the algorithms employed are tested.

Keywords: visco-hypoelasticity model, Kirchhoff stress tensor, Hencky strain tensor, Green-Naghdi rate.

1 Introduction

The materials are termed viscoelastic because they exhibit both solid- and fluid-like behaviour, and amongst examples of such media we find concrete and the thermoplastic polymers. The polymers consist of so called long chain molecules. They are easily moulded, lightweight and may be made strong plastics. The long chains, or backbones, are constructed by joining a great many hydrocarbon monomers together to form periodic sequences of specific arrangements of hydrogen and carbon atoms; this is then the long chain, the polymer.

Solid polymers can occur in the amorphous or crystalline state. Polymers in the amorphous state are characterized by a disordered arrangement of the macromolecular chains, which adopt conformations corresponding to statistical coils. The crystalline state is characterized by a long-range three dimensional order (order extending to distances of hundreds or thousands of times the molecular size of the

repeating unit). The macromolecular chains in this state adopt fixed conformations such as planar zigzag, or helical. These chains are aligned parallel to each other, forming a compact packing that gives rise to a three-dimensional order. Many polymers have the capability to crystallize. This capability basically depends on the structure and regularity of the chains and on the interactions between them. The term "semicrystal1ine state" should be used rather than crystalline state, because regions in which the chains or part of them have an ordered and regular spatial arrangement coexist with disordered regions typical of the amorphous state.

Viscoelastic behavior is typical of a number of materials such as polymers and plastics, as explained previously. These materials have memory, i.e. the stress depends on the entire history of the deformation and typically this memory fades with time. In dual formulation the strain can be represented as a functional of the stress history which, due to the requirement that the principle of material objectivity needs to be satisfied. This leads to reasonably complex relations even in the "simplest" of constitutive relations.

Later in this paper it describes a dual finite visco-hypoelastic model based in Hencky strain measure used in small strain contexts to the case of large deformation. The extension to the large deformation case is achieved by considering

a multiplicative decomposition of the deformation gradient and taking the logarithm strain measure with rotated Kirchhoff stress as the conjugated pair. Before presenting the model, this paper begins with a brief discussion about basic physical phenomena of creep and stress relaxation, typical for viscoelastic materials. The subsection 2.2 starts by a discussing the two more general categories of viscoelastic constitutive models: integral and differential models. In the subsection 2.3 are presented the derivation of our dual integral constitutive model. The section 3 presents the strong, weak (variational) formulation of the problem the numerical scheme. Finally the section 4 discusses the numerical applications.

2 Constitutive laws

Viscoelastic media are characterized by two basic phenomena: creep and stress relaxation. We consider both cases below.

2.1 Creep and relaxation

Consider a simple uniaxial bar of a viscoelastic material, subjected to an instantaneously applied and sustained tensile load as shown in figure 1.

Firstly imagine a qualitatively similar bar, again fixed at one end, to which an on/off axial step loading is applied at the other, that is, at $t_0 = 0$ the loading increases instantaneously to the constant value F and at $t^* > t_0$, F is removed as illustrated in figure. The bar now responds by extending in length and we denote this extension by u(t). At the instant t_0 + there is again linear elastic behaviour and $u(t_0+)$ is therefore given by Hooke's law, but over the range $t \in (t_0, t^*)$, the bar will continue to extend, this behaviour is termed creep. If for arbitrarily large t^* this creep continues indefinitely then the material is a viscoelastic fluid, on the other hand if u(t) approaches some constant value



Figure 1: Schematic creep

then it is a viscoelastic solid. Upon removal of the load F at $t = t^*$ the material again displays elastic behaviour, there is an elastic recovery where u instantaneously snaps back to a lesser value.

Thereafter is another creep phase during which the material attempts to return to its original configuration. It can make a solid fluid distinction: if, as $t \to \infty$ we have $u \to 0$ then the material is a solid but if $u \to constant \neq 0$ then there is a permanent set within the bar caused by irreversible molecular flow during the initial creep phase and the material is a fluid.

The ability of a viscoelastic material to attempt to return to its original configuration even after inelastic deformation has taken place implies that it somehow has an internal record of its initial state. If this is the case then it seems plausible that it also keeps a record of all of its states up to the present time and for this reason viscoelastic materials are said to possess memory.

Now we think of the bar as being fixed rigidly at one end and, at some reference time t = 0, an instantaneous longitudinal displacement u, applied to the other as schematically shown in the figure 2.

In response an internal longitudinal stress σ is set up within the bar which at the instant, t = 0+, is given by Hooke's law, and so the instantaneous response of the material is linear elastic. Over time however the stress decreases monotonically to either the constant, nonzero, value σ_0 or to zero. In the former case the material is termed a viscoelastic solid whilst in the latter a viscoelastic fluid. This phenomena is known as stress relaxation.



Figure 2: Schematic stress relaxation

2.2 Linear visco-hypoelastic constitutive model

As we have seen for an elastic solid, the stress is determined by the deformation of the material relative to a fixed reference configuration. However, it is. One blank line must be included above and bellow each equation. evident that several materials, exhibit viscoelastic characteristics, i.e. the magnitude of the measured stress depends on strain, strain rate, time and temperature as well, although we will not consider it here. In this sense the stress in viscoelastic materials can be represented as a functional of the history of the deformation. In other words, these materials have memory: the stress depends on the entire history of the motion, and typically this memory fades with time. There are a number of approaches for constructing constitutive models for the large strain viscoelastic deformation. Mathematical relations which describe how stress can depend on the history of the deformation are either given in integral form or in differential form. In integral form the stress at time t is given in terms of an expression which involves an integral over previous times. The integral in such an expression is known as a history integral. In contrast, the differential form of constitutive model the history of the deformation is taken into account by certain ordinary differential equations which describe how certain quantities known as internal variables evolve in time. For a more detailed presentation of both ways of representing viscoelastic constitutive models see, for example see the references Drozdov [1], Haupt [2], Johnson *et al.* [3], Reismann and Pawlik [4] and Truesdell and Noll [5].

The Boltzmann superposition principle follows by that in each strain step the stress evolution is given by Hooke's law. In this sense, the evolution in each strain step component is approximated with

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a piecewise continuous step function. For sufficiently smooth fields, the general linear constitutive equation for the linear viscoelastic (small deformation) solid is given by

$$\sigma_{ij}(t) = D_{ijkl}(t - t_0)\varepsilon_{kl}(t_0) + \int_{t_0}^t D_{ijkl}(\mathbf{t} - \xi)\dot{\varepsilon}_{kl}(\xi)d\xi$$
(1)

or equivalently

$$\sigma_{ij}(t) = D_{ijkl}(t_0)\varepsilon_{kl}(t-t_0) - \int_{t_0}^t \dot{D}_{ijkl}(\mathbf{t}-\xi)\varepsilon_{kl}(\xi)d\xi$$
(2)

Considering now a viscoelastic isotropic material

$$D(t) = 2G(t)II_{DEV} + K(t)(I \otimes I)$$
(3)

in which

$$II_{DEV} = II - \frac{1}{3}(I \otimes I) \tag{4}$$

where I is the second order identity tensor and II is the fourth order identity tensor and the kernel functions are represented in terms of Prony series, which assumes that:

$$G(t) = G_{\infty} + \sum_{i=1}^{n_G} G_i \exp\left(-\frac{1}{\tau_i^G}\right)$$
(5)

$$K(t) = K_{\infty} + \sum_{i=1}^{n_K} K_i \exp\left(-\frac{1}{\tau_i^K}\right)$$
(6)

in which G_{∞} and G_i are shear elastic moduli, K_{∞} and K_i are bulk elastic moduli and τ_i^G and τ_i^K are the relaxation times for each Prony component. An a alternative formulation for the quasi-static rate model is the constitutive equation given in

$$\varepsilon_{ij}(t) = C_{ijkl}(t - t_0)\sigma_{kl}(t_0) + \int_{t_0}^t C_{ijkl}(\mathbf{t} - \xi)\dot{\sigma}_{kl}(\xi)d\xi$$
(7)

in which

$$C = \frac{B}{9}(I \otimes I) + \frac{J}{2}II_{DEV}$$
(8)

where B is the bulk compliance function and J is the shear compliance function with the kernel functions are represented in terms of Prony series, which assumes that:

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$$B(t) = B_0 + \sum_{i=1}^{n_G} B_i \left(1 - \exp\left(-\frac{1}{\tau_i^B}\right) \right)$$
(9)

$$J(t) = J_0 + \sum_{i=1}^{n_G} J_i \left(1 - \exp\left(-\frac{1}{\tau_i^J}\right) \right)$$
(10)

in which J_0 and J_i are shear compliance moduli, B_0 and B_i are bulk compliance moduli and τ_i^B and τ_i^J are the relaxation times for each Prony component.

2.3 Finite visco-hypoelastic constitutive model

The Hencky's logarithmic strain measure model was proposed in 1938 to study elastic behaviour of rubbers at some simple finite deformation modes. The Hencky's logarithmic strain or natural strain has inherent advantages over other strain measures in his study of a priori constitutive inequalities and treated the Hencky strain, its rate and its work-conjugate stress as basic measures for strain, strain rates and stresses. The Hencky's logarithmic tensor E, based in Lagrangean formulation, can be defined in following way:

$$E(x_o, t) = \frac{1}{2} \ln (C(x_o, t));$$

= ln (U(x_o, t)) (11)

where U is the symetric positive defined second order tensor from polar decomposition of F = RU (gradient of the deformation function). From the spectral decomposition:

$$U(x_o, t) = \sum_{i=1}^n \sqrt{\Lambda_i} \left(\varphi_i \otimes \varphi_i\right) \tag{12}$$

with $\{\Lambda_i\}_{i=1}^n$ and $\{\varphi_i\}_{i=1}^n$ are the eigenpairs of C. As pointed out by the famous Hill's work in 1978, the rate of stress work per unit of mass which is invariant under a change of strain measure and the reference configuration is used

to generate stress measures conjugate to the family of strain measures

$$\dot{W} = \frac{1}{\rho} \left(\sigma : D \right) = \frac{1}{\rho_o} \left(\tau : D \right) = \frac{1}{\rho_o} \left(P : \dot{F} \right) = \frac{1}{2\rho_o} \left(S : \dot{C} \right)$$
(13)

in which σ is the Cauchy stress tensor, τ is the Kirchhoff stress tensor, D is the infinitesimal deformation rate, P is the first Piola-Kirchhoff stress, F is the gradient of the deformation function, S is the second Piola-Kirchhoff stress, C is the right Cauchy-Green strain tensor and ρ_o and ρ being the reference and the current mass densities. Then, one follows that

Theorem 1 The rotated Kirchhoff stress tensor ($\bar{\tau} = R^T \tau R$) forms the conjugated stresstensor pair with the Hencky's logarithmic strain measure (E), under the isotropy hypothesis, i.e.

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$$\dot{W} = \frac{1}{\rho_o} \left(\bar{\tau} : \dot{E} \right) \tag{14}$$

Proof We have

$$\rho_o \dot{W} = \tau : D = \bar{\tau} : \left(R^T D R \right)$$

Thus observing that $R^T D R$ can be rewritten as follow

$$R^T D R = \frac{1}{2} \left(U^{-1} \dot{U} + \dot{U} U^{-1} \right).$$

From the spectral decomposition, we have

$$\dot{E} = \frac{1}{2} \sum_{i=1}^{n} \left[\frac{\dot{\Lambda}_{i}}{\Lambda_{i}} \left(\varphi_{i} \otimes \varphi_{i} \right) + \ln\left(\Lambda_{i}\right) \left(\dot{\varphi}_{i} \otimes \varphi_{i} + \varphi_{i} \otimes \dot{\varphi}_{i} \right) \right]$$

and observing that $\varphi_i : \varphi_j = \delta_{ij}$ and $\dot{\varphi}_i : \varphi_i = \varphi_i : \dot{\varphi}_i = 0$, we conclude that

$$\tau: D = \bar{\tau}: \dot{E}.\tag{15}$$

By a similar way it follows in this unrotated configuration the constitutive equation may be rewritten as

$$E(t) = \bar{C}(t - t_0)\bar{\tau}(t_0) + \int_{t_0}^t \bar{C}(\mathbf{t} - \xi)\dot{\tau}(\xi)d\xi$$
(16)

In order to generalize this constitutive equation to finite deformation problems, it is necessary to introduce the following definition

Definition 1 Let be v, A, and H (first order, second order and fourth order tensor respectively), one defines the pull back or bar transformation as

$$\bar{v}(t) = \Theta^T(t) \, v(t) \tag{17}$$

$$\bar{A}(t) = \Theta^{T}(t) A(t) \Theta(t)$$
(18)

$$\bar{H}(t) = \Theta^{T}(t) \Theta^{T}(t) H(t) \Theta(t) \Theta(t)$$
(19)

and from continuum mechanics

$$\bar{F}(t) = \Theta^T(t) F(t) \tag{20}$$

$$\bar{C}(t) = \Theta^T(t) C(t) \Theta(t)$$
(21)

These pull back (rotation neutralized) quantities with $\Theta(t)$ are used to define a convenient framework to perform the integration of the constitutive model. Indeed, the pull back Kirchhoff stress tensor can be defined as

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$$\bar{\tau}(t) = \Theta^T(t)\,\tau(t)\,\Theta(t) \tag{22}$$

and one can show that

$$\dot{\bar{\tau}}(t) = \Theta^T(t) \, \breve{\tau}(t) \, \Theta(t) \tag{23}$$

(for proof details see the reference Azikri de Deus [6]) where $\tau^{:}(t)$ denotes the Green-Naghdi rate of the pull back Kirchhoff stress tensor, which is given by

$$\dot{\tau} = \dot{\tau} - \Xi \tau + \tau \Xi \tag{24}$$

where $\Xi(t) = \dot{R}(t) R^{T}(t)$ (spin tensor). Let us define the rotation tensor $\Theta(t)$, as the solution to the following initial value problem:

Problem 1 Given $\Xi(t)$, find $\Theta(t)$ that solves

$$\dot{\Theta}(t)\,\Theta^T(t) = \Xi(t) \tag{25}$$

$$\Theta(t) = \Xi(t)\,\Theta(t) \tag{26}$$

$$\Theta(0) = I \tag{27}$$

By simple observation, one can verify that the solution to the initial value problem is given by $\Theta(t) = R(t)$ (for more details see the references Azikri de Deus [6] and Truesdell and Noll [5]).

3 The finite visco-hypoelastic problem

The approach used here is the total Lagragian formulation. Considering the reference configuration Ω_o , defined at t_o , a bounded domain with a Lipschitz boundary $\partial \Omega_o$ subjected to a body force b defined on Ω_o , a prescribed surface traction defined on Γ_o^t and a prescribed displacement defined on Γ_o^u , where $\partial \Omega_o = \overline{\Gamma_o^t} \cup \overline{\Gamma_o^u}$ and $\Gamma_o^t \cap \Gamma_o^u$.

Taking the motion function $\phi_t : \Re^3 \to \Re^3$ such that $x = \phi(x_o, t) = \phi_t(x_o)$ $\therefore x_o = \phi_t^{-1}(x)$. It follows that the displacement field is defined as: $x = u(x_o, t) + x_o$ $\therefore u_o(x_o, t) = \phi_t(x_o) - x_o = x - x_o = x - \phi_t^{-1}(x) = u(x_o, t)$. Thus, it is possible to announce the problem in the reference configuration as: **Problem 2** For each $t \in [0, t_f]$ determine $u_o(x_o, t)$ that solves the following boundary value problem stated as

$$\operatorname{div} P(x_o, t) + \rho_o(x_o) b(x_o, t) = 0 \quad \operatorname{in} \quad \Omega_o$$

$$\tag{28}$$

$$P(x_o, t) n_o(x_o, t) = \bar{t}_o(x_o, t) \qquad in \quad \Gamma_o^t$$
(29)

$$u_o(x_o, t) = \bar{u}_o(x_o) \qquad \qquad in \quad \Gamma_o^u \tag{30}$$

with $b(x_o, t) \in L_2(\Omega_o)$ and $\bar{u}_o(x_o) \in H_{00}^{1/2}(\Gamma_o^u)$ for each $t \in [0, t_f]$.

Let us define now the following sets, for each time $t \in [0, t_f]$

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$$Kin_o^u = \left\{ u_o : \Omega_o \to \Re^3 \left| u_o \in H^1\left(\Omega_o\right), \, u_o(x_o, t) = \bar{u}_o(x_o) \, in \, \Gamma_o^u \right\}$$
(31)

$$Var_o^u = \left\{ \hat{v} : \Omega_o \to \Re^3 \left| \hat{v} \in H^1(\Omega_o), \, \hat{v}(x_o) = 0 \text{ in } \Gamma_o^u \right. \right\}$$
(32)

Thus it has the weak form of the problem

Problem 3 For each $t \in [0, t_f]$ determine $u_o(x_o, t) \in Kin_o^u$ such that

$$\int_{\Omega_o} P : \nabla \hat{v} \, d\Omega_o = \int_{\Omega_o} \rho_o b \cdot \hat{v} \, d\Omega_o \, + \, \int_{\Gamma_o^t} \bar{t}_o \cdot \hat{v} \, d\partial\Omega_o, \,\,\forall \hat{v} \in Var_o^u \tag{33}$$

For each $t \in [0, t_f]$, it can denoting

$$\Im(u_o; \hat{v}) = \int_{\Omega_o} P: \nabla \hat{v} \, d\Omega_o - \int_{\Omega_o} \rho_o b \cdot \hat{v} \, d\Omega_o - \int_{\Gamma_o^t} \bar{t}_o \cdot \hat{v} \, d\partial\Omega_o, \ \forall \hat{v} \in Var_o^u$$
(34)

Then, the problem can be stated as

Problem 4 For each $t \in [0, t_f]$ determine $u_o(x_o, t) \in Kin_o^u$ such that

$$\Im\left(u_o;\hat{v}\right) = 0, \ \forall \hat{v} \in Var_o^u \tag{35}$$

The problem above is approached by Newton method in association with Galerkin-FEM, and the incremental formulation follows from the schematic algorithm in Tab. 1

Table 1: Newton's Method Algorithm – Incremental Formulation.

For each time step $t = t_n$; (i) Initialize the iteration counter $k \leftarrow 0$; (ii) Initialize the variable vector $u_{n+1}^0 = u_n$; (iii) Compute the residue vector, error = $\|residue vector\|$; (vi) Do while (error > tolerance¹) (1) Determine the tangent modulus $\left[\aleph(u_{n+1}^k)\right]_{ijkl} = \frac{\partial P_{ij}}{\partial F_{kl}}\Big|_{u=u_{n+1}^k}$ (2) Solve the problem $\int_{\Omega_o} \aleph(u_{n+1}^k) \nabla(\Delta u_{n+1}^k) : \nabla \hat{v} d\Omega_o = -\Im\left(u_{n+1_o}^k; \hat{v}\right), \ \forall \hat{v} \in Var_o^u$; (3) Actualize the variable vector $u_{n+1}^{k+1} = u_{n+1}^k + \Delta u_{n+1}^k$; (4) Compute the new error; (5) Actualize $\Im\left(u_{n+1}^k; \hat{v}\right) \leftarrow \Im\left(u_{n+1}^{k+1}; \hat{v}\right) \text{ and } k \leftarrow k+1$; End Do while.

⁽¹⁾: previously defined.

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4 Numerical examples

For these applications, one used a mesh with two six points triangular elements. The developed code is written in Fortran 90 and for post processing, it's used the GID 8.0 software. The global tolerance is 10^{-6} .

EXAMPLE 1: In this example, one is considered the plane strain state. The body is a rectangular shape, in which the dimentions are width $1 (\times 25, 4 mm)$ and height $2 (\times 25, 4 mm)$. Let be presented the following reference configuration $\Omega_o = \{(x, y) | 0 < x < 1 (\times 25, 4 mm) \text{ and } 0 < y < 1 (\times 25, 4 mm)\}$ under symmetry considerations. For the quasi-static problem one has the boundary conditions: $\bar{u}_x(0, y, t) =$ $\bar{u}_y(0, y, t) = 0$, $\bar{u}_x(1, y, t) = 0.1 t (\times 25, 4 mm)$ and the other conditions are tension free for $t \in [0, 1]$ (see fig. 3). In this example one demonstrates the consistence of the numerical algorithm (code) by comparing the numerical solution against artificial exact solution. Invariably one design the loads and tractions so that the exact stretch have the form $x(t) = \lambda_1(t) x_o$ and $y(t) = \lambda_2(t) y_o$.



Figure 3: Traction test.

By a simple computation from the boundary condition and supposing

$$J(t) = 3,2386 \times 10^{-8} \left(1 - e^{\frac{1}{20,2599}t} \right) + 5,8578 \times 10^{-7} \left(\times 6,89 \, kPa \right)^{-1} \tag{36}$$

one has that this block is composed by a polymer that has the following ralaxation function for B

$$B(t) = 4,7279 \times 10^{-8} \left(1 - e^{\frac{1}{19,8283}t} \right) + 8,7867 \times 10^{-7} \left(\times 6,89 \, kPa \right)^{-1}$$
(37)

where the time scale is taken in days. In next figure (see fig. 4), one presents the time evolution of σ_{xx} in the body (constant profile along entire body).

One can observe the evolution of stress σ_{xx} component with the time for one day observation. Note that the numerical results are equal to the exact solution of the problem for each time step. The last figure shows the displacement profile on the deformed body (see fig. 5).



Figure 4: Tension (kPa) vs. time (days).



Figure 5: Displacement for t = 1 day.

EXAMPLE 2: In this example, one is considered the plane strain state. The body is a square shape $(2 (\times 25, 4 mm) \times 2 (\times 25, 4 mm))$ with a circular hole inside (radius = $0, 2 (\times 25, 4 mm)$). This hole is placed at the geometrical center of square shape. For the quasi-static problem, the body is submitted to prescribed displacement conditions on right and left (same value) side of the square shape and the other conditions are free stress. Motivated by numerical effort reduction, this problem is approached under simety considerations (1/4 of geometry - see fig. 6).

On the right side one has $\bar{u}_x(1, y, t) = 0.1 t (\times 25, 4 mm)$ for $t \in [0, 1]$. The polymer is the same of

example 1 where the time scale is taken in days. In this example one is used 801 elements and 1682 nodes (see fig. 7).



Figure 6: 1/4 Square shape with a circular hole.



Figure 7: Tri 6 elements mesh.

The figure 8 shows the displacement field at the final observation instant. The figure 9 shows the stress σ_{xx} profile. Note that high stress levels are in top of the central hole. The figure 10 shows the

stress σ_{xy} profile, where higher stress levels are in top of the central hole and in the figure 11 is exposed the stress σ_{yy} profile. The high stress levels are too in top of the central hole.



Figure 8: Displacement for t = 1 day.







Figure 10: σ_{xy} profile for t = 1 day.



Figure 11: σ_{yy} profile for t = 1 day.

EXAMPLE 3: In this example, one is considered the plane strain state. The body is a complex geometry component (dimensions in inches). For the quasi-static problem, this body is submitted to prescribed displacement conditions on right side and the others condition are free stress conditions (see fig. 12).

On the right side one has $\bar{u}_x(1, y, t) = -0, 3t (\times 25, 4mm)$ for $t \in [0, 1]$. The polymer is the same of examples 1 and 2, where the time scale is taken in days. In this example one is used 337 elements and 755 nodes (see fig. 13).

The figure 14 shows the displacement field at the final observation instant. The figure 15 shows the stress σ_{xx} profile. Note that high stress levels are in upper right and low left of the central hole. The figure 16 shows the stress σ_{xy} profile, where higher stress levels are in upper right and low left of the central hole. In the figure 17 is exposed the stress σ_{yy} profile. The high stress levels are in upper left and low right of the central hole.



Figure 12: Problem sketch.



Figure 13: Tri 6 elements mesh.



Figure 14: Displacement for t = 1 day.



Figure 15: σ_{xx} profile for t = 1 day.



Figure 16: σ_{xy} profile for t = 1 day.



Figure 17: σ_{yy} profile for t = 1 day.

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