On the modeling of the linear viscoelastic behaviour of biological materials using Comsol Multiphysics

F. Moravec\textsuperscript{a,}*, N. Letzelter\textsuperscript{b}

\textsuperscript{a}Faculty of Applied Sciences, UWB in Plšen, Univerzitní 22, 306 14 Plzeň, Czech Republic
\textsuperscript{b}ISBS, University Paris 12, 8 rue du Général Sarrail, 94010 Créteil, France

Received 23 August 2007; received in revised form 4 October 2007

Abstract

The aim of this article is to simulate the viscoelastic behaviour during quasi-static equilibrium processes using the software Comsol Multiphysics. Two-dimensional constitutive equations of the three most classical rheological models (the Kelvin-Voigt, Maxwell and Three-Elements models) are developed and the mechanical equations for each model are rewritten to be compatible with the predefined Comsol format in the so-called Coefficients mode. Results of the simulations on creep and relaxation tests are compared with experimental data obtained on a sample of biological tissue.

\textcopyright 2007 University of West Bohemia. All rights reserved.

Keywords: viscoelasticity, mechanical equilibrium, Comsol modeling

1. Introduction

Viscoelastic behaviour is characteristic of numerous materials, as polymers and biological tissues for instance. Restricting our study under the hypothesis of small perturbations, rheological models can be developed to catch the (linear approximation of the) materials mechanical behaviour. These rheological models are classically represented as combinations of elastic elements (springs) and viscous elements (dashpots) distributed in parallel or series branches. In this paper, we focus on the three most classical models: the so-called Kelvin-Voigt, Maxwell and Three-Elements models. The aim of this article is to simulate their mechanical behaviour during quasi-static equilibrium processes using the software Comsol Multiphysics. That software is designed for solving a system of differential equations coupled with boundaries conditions and initial solutions. Even if the solution is based on the finite elements method, the differential equations can be entered in their strong form but the user has to respect conventions of inputting equations (see section 4). Material behaviour is simulated both on creep and relaxation tests, and results of the simulations are compared with experimental data obtained on a sample of smooth muscle extracted from a gastropod intestine.

*Corresponding author. Tel.: +420 377 364 825, e-mail: fanny@kme.zcu.cz.
2. Constitutive equations

The constitutive equation for (compressible, isotropic, linear) elastic behaviour is usually written as

$$\sigma = R \epsilon, \quad (1)$$

where the rigidity tensor $R$ is defined in dependence on the Young modulus $E$ and on the Poisson coefficient $\nu$, i.e.

$$R = \begin{pmatrix} 1/E & -\nu/E & 0 \\ -\nu/E & 1/E & 0 \\ 0 & 0 & (1 + \nu)/E \end{pmatrix}, \quad (2)$$

considering the two-dimensional space. Similarly, the constitutive equation for (compressible, isotropic, linear) viscous behaviour can be written as

$$\sigma = Q \dot{\epsilon}, \quad (3)$$

where $Q$ is defined in dependence on the viscosity modulus $\eta$ and on the compressibility coefficient $\kappa$, i.e.

$$Q = \begin{pmatrix} 1/\eta & -\kappa/\eta & 0 \\ -\kappa/\eta & 1/\eta & 0 \\ 0 & 0 & (1 + \kappa)/\eta \end{pmatrix}, \quad (4)$$

Viscoelastic behaviour is schematized as combinations of elastic (springs) and viscous (dashpots) elements. Elements can be combined in parallel or in series, see fig. 1. By extension of the well-known one-dimensional rheological models [2][5], we develop constitutive equations for two-dimensional schemas where elastic and viscous elements’ behaviours are governed by (1) and (3) respectively. The two-elements figure combining a dashpot and a spring in parallel is the *Kelvin-Voigt* model (abbreviation: KV). It is led by the constitutive equation

$$\sigma = R \epsilon + Q \dot{\epsilon}, \quad (KV \ model). \quad (5)$$

The two-elements figure combining a dashpot and a spring in series is the *Maxwell* model (abbreviation: MX). It is led by the constitutive equation

$$\dot{\epsilon} = R^{-1} \sigma + Q^{-1} \dot{\sigma}, \quad (MX \ model). \quad (6)$$

The *three-elements* model (abbreviation: TE) combining a spring in series with parallel branches containing a spring and a dashpot respectively is also studied. It is led by the constitutive equation

$$R_A Q \dot{\epsilon} + R_A R_B \epsilon = Q \dot{\sigma} + (R_A + R_B) \sigma, \quad (TE \ model). \quad (7)$$
3. Mechanical equations

We consider a material sample having the two-dimensional geometry $\Omega$ (for instance, a rectangle of dimensions $l \times L$). That sample is submitted to mechanical loading through boundary conditions on $\partial \Omega$. The problem of quasi-static equilibrium can be written as: Find the fields of displacement, $u(x, y, t)$ and $v(x, y, t)$, fulfilling:

$$
\begin{align*}
\text{the behaviour law, } & F(\sigma, \dot{\sigma}, \epsilon, \dot{\epsilon}) = 0, \text{ in } \Omega, \\
\text{the equilibrium equation, } & \text{div} \sigma = 0, \text{ in } \Omega, \\
\text{the boundary conditions on } & \partial \Omega, \\
\text{the initial solution at } & t = 0 \text{ in } \Omega.
\end{align*}
$$

(8)

A material sample is tested with a traction machine, see fig.2. The loading is applied on the up border while the position of the down one is maintained by the condition $v|_{y=0} = 0$, $\forall x$, $\forall t$. The distribution of deformation within the sample is assumed to be symmetric with respect to the centered vertical axis: During numerical simulations, we consider the only right half of the sample (the domain $\Omega$) and we apply the condition $u|_{x=0} = 0$, $\forall y$, $\forall t$, on the left border. The remained border is assumed to be free of stress: $\sigma_{11}|_{x=l} = 0$, $\forall y$, $\forall t$. Simulations are done both on the creep test (i) and on the relaxation (ii) test:

(i) At the time $t = 0$, an instantaneous force is applied on the up boundary and that force is held constant in time: $\sigma_{22}|_{y=L} = f$, $\forall x$, $\forall t$.

(ii) At the time $t = 0$, an instantaneous strain is imposed by moving the up border and that deformation is held constant in time: $v|_{y=L} = \delta$, $\forall x$, $\forall t$.

![Fig. 2. Mechanical traction test.](image-url)
4. Comsol modeling in mode ‘Coefficient’

In Comsol’s language, the so-called Coefficient mode is best adapted for solving linear differential equations [1]. It is used to input the equations of the problem respecting the following scheme:

\[
\begin{align*}
&ea \frac{\partial^2 U}{\partial t^2} + da \frac{\partial U}{\partial t} + \nabla \cdot (-c \nabla U - al U + ga) + be \cdot \nabla U + a \ U = f \quad \text{in } \Omega, \\
&n \cdot (c \nabla U + al U - ga) + q \ U = g - h^T \mu, \quad \text{on } \partial \Omega \text{ (Neuman condition)}, \\
&h \ U = r, \quad \text{on } \partial \Omega \text{ (Dirichlet condition)},
\end{align*}
\]

(9)

where
- \(U\) is the vector of unknown variables,
- \(ea, da, c, al, ga, be, f, q, g, h\) and \(r\) are tensors (of various orders, and of which the dimensions depend on the dimension of the vector \(U\) and on the space dimension) collecting the material coefficients,
- \(h^T\) is the transposed of \(h\),
- \(n\) is the unitary normal output vector on the considered boundary,
- \(\mu\) is a Lagrange multiplicator Lagrange mixing Neuman and Dirichlet conditions on the considered boundary [1].

Comsol programs can be translated in Matlab language. Information is then stoked in a Matlab structure, the so-called fem. structure [1]. For instance, information on the unknown vector in stocked in the field fem.dim, on the differential equation in the fields fem.equ.ea .. fem.equ.f, on the boundaries equations in the fields fem.bnd.q .. fem.bnd.r, and on the initial solution in the field fem.equ.init.

The main part of the Comsol modeling consists of identifying the coefficients’ tensors \(ea, da, c, al, ga, be, f, q, g, h\) and \(r\) by comparing the mechanical equations (8) with the Comsol ones (9). In two-dimensional elasticity, the dimension of the problem is given by the definition of the vector of unknown variables: \(U = (u, v)\) where \(u\) and \(v\) are the components of the displacement field along the two spatial directions. Since we have two unknown variables, we must have two (differential) equations: They are given by the projections of the equilibrium equation, \(\text{div} \sigma(U) = 0\), on the space axis, where \(\sigma(U)\) is replaced by the elastic behaviour law (1). In opposition to this, when studying viscoelastic materials, we meet the following difficulties:

(i) Coupled time-space derivatives of the type \(\frac{d}{dt} \frac{\partial U}{\partial x}\) do not (explicitly) occur in the Comsol system (9) while we need them in the mechanical equations (8).

(ii) For the models of type Maxwell and Three-Elements we are not able to extricate the \(\sigma\)-expression from the constitutive law, because the later is a differential equation for \(\sigma\). Consequently, we cannot replace \(\sigma\) by the behaviour law when writing the projection of \(\text{div} \sigma(U) = 0\) on the space axis.

To bypass these difficulties we enrich the number of degrees of freedom as following:

(i) New variables, \(b\) and \(p\), are added within the \(U\)-definition. In parallel we define two
adding equations: $\dot{u} - b = 0$ and $\dot{v} - p = 0$. Consequently, the hybrid derivatives, e.g. $\frac{d}{dt} \frac{\partial u}{\partial x}$, reduce to purely spatial derivatives, e.g. $\frac{\partial r}{\partial x}$.

(ii) The three components of the stress $\sigma_{11}$, $\sigma_{22}$ and $\sigma_{12}$ are input as new variables (enriching the $U$-definition). In parallel the number of differential equations to be solved by Comsol Multiphysics is increased by adding the components of the behaviour equation (three scalar expressions) to the projections of the equilibrium equation.

Rewritten mechanical equations (8) in respect with the Comsol format (9) are given in tab. 1. For instance, the developed equations for the Three-Elements model are

$$\begin{align*}
\Phi \frac{\partial \sigma_{11}}{\partial t} + \kappa \Phi \frac{\partial \sigma_{22}}{\partial t} + A \sigma_{11} + B \sigma_{22} - D \frac{\partial b}{\partial x} - E \frac{\partial p}{\partial y} - G \frac{\partial u}{\partial x} - H \frac{\partial v}{\partial y} &= 0, \\
\kappa \Phi \frac{\partial \sigma_{11}}{\partial t} + \Phi \frac{\partial \sigma_{22}}{\partial t} + B \sigma_{11} + A \sigma_{22} - E \frac{\partial b}{\partial x} - D \frac{\partial p}{\partial y} - H \frac{\partial u}{\partial x} - G \frac{\partial v}{\partial y} &= 0, \\
\frac{\eta}{1 + \kappa} \frac{\partial \sigma_{12}}{\partial t} + C \sigma_{12} - F \frac{\partial b}{2 \partial y} - F \frac{\partial p}{2 \partial x} - I \frac{\partial u}{2 \partial y} - I \frac{\partial v}{2 \partial x} &= 0,
\end{align*}$$

where $\Phi$, $A$ .. $I$ are function of the material coefficients:

$$\Phi = \frac{\eta}{1 - \kappa^2}, \quad \Delta_A = \frac{E_A}{1 - \nu_A^2}, \quad \Delta_B = \frac{E_B}{1 - \nu_B^2},$$

$$A = \Delta_A + \Delta_B, \quad B = \nu_A \Delta_A + \nu_B \Delta_B, \quad D = \Delta_A \Phi(1 + \nu_A \kappa),$$

$$E = \Delta_A \Phi(\nu_A + \kappa), \quad G = \Delta_A \Delta_B(1 + \nu_A \nu_B), \quad H = \Delta_A \Delta_B \nu_A + \nu_B,$$

$$C = \frac{E_A}{1 + \nu_A} + \frac{E_B}{1 + \nu_B}, \quad F = \frac{(1 + \kappa)(1 + \eta_A)}{(1 + \eta_A)(1 + \eta_B)}, \quad I = \frac{\eta E_A E_B}{(1 + \eta_A)(1 + \eta_B)}.$$

Confronting the system (10) with the predefined Comsol’s system (9) we observed that only the tensors $a_l$, $b$, $da$, $a$, $g$, $h$ and $r$ are not zero. Their expressions are detailed in [4]. The tensors $g$, $h$, $r$, are related to the boundary conditions. Because of the increase of the number of degrees of freedom, the Dirichlet conditions on $u$ or $r$ have to be enriched by conditions on $b$ or $p$, respectively. That is $b|_{x=0} = 0$, $\forall y$, $\forall t$ and $p|_{y=0} = 0$, $\forall x$, $\forall t$. Moreover, when simulating relaxation test, $p|_{y=L} = 0$, $\forall x$, $\forall t$.

Initial solution is needed for every variable in which time derivative is involved in modeling equations. Consequently, initial condition is needed on $u$ and $v$ for the Kelvin-Voigt model; on each $\sigma_{ij}$, $i, j = 1, 2$ for the Maxwell model; and on $u$, $v$ and $\sigma_{ij}$, $i, j = 1, 2$ for the Three-Elements model. Nevertheless, the initial solutions must be compatible with the boundary conditions. In every case they are needed, we fix $\sigma_{11}^{init}(x, y)$ and $\sigma_{12}^{init}(x, y)$ as zero. Also, we
\[
\begin{bmatrix}
    u \\
    v \\
    b \\
    p
\end{bmatrix}
\]
\[
\nabla (R \epsilon(u, v) + Q \dot{\epsilon}(b, p)) = 0,
\]
\[
\dot{u} - b = 0 \quad \text{and} \quad \dot{v} - p = 0.
\]

\[
\begin{bmatrix}
    b \\
    p \\
    \sigma_{11} \\
    \sigma_{22} \\
    \sigma_{12}
\end{bmatrix}
\]
\[
\nabla \sigma = 0,
\]
\[
\dot{\epsilon}(b, p) = R^{-1} \sigma + Q^{-1} \sigma.
\]

\[
\begin{bmatrix}
    u \\
    v \\
    b \\
    p \\
    \sigma_{11} \\
    \sigma_{22} \\
    \sigma_{12}
\end{bmatrix}
\]
\[
\nabla \sigma = 0,
\]
\[
\dot{u} - b = 0 \quad \text{and} \quad \dot{v} - p = 0,
\]
\[
R_A Q \dot{\epsilon}(b, p) + R_A R_B \epsilon(u, v) = Q \sigma + (R_A + R_B) \sigma.
\]

Tab. 1. Compatible equations with the Comsol coefficient mode for the three viscoelastic models.

Assume the initial components of the displacement of the form

\[
u^{\text{init}}(x, y) = \epsilon_{11}^{\text{init}} x \quad \text{and} \quad v^{\text{init}}(x, y) = \epsilon_{22}^{\text{init}} y.
\]

When simulating the creep test we fix \(\sigma_{22}^{\text{init}}(x, y) = f, \forall x, \forall y\). When simulating the relaxation test we fix \(\epsilon_{22}^{\text{init}}(x, y) = \delta/L, \forall x, \forall y\). There is no restriction on the remaining initial solutions: The user has to input them by the same way as he has to input the material coefficients \(E_A\) – see the summary of free model parameters in tab. 2. Note finally that the Maxwell model does not work with the variables \(u\) and \(v\) because \(\epsilon\) is not involved in the constitutive equation. As a consequence, results are obtained in term of rate displacement only (that the user may integrate by himself to obtain information on the displacement field).

5. Results

Since material is assumed to be homogeneous and the loading tests are of the type ‘traction test’, numerical simulations confirm without surprise that the extra-diagonal terms \(\sigma_{12}\) and \(\epsilon_{12}\) are zero, and that the distributions of \(\sigma_{ii}\) and \(\epsilon_{ii}\) are constant in space. Thus, \(\sigma_{11} = 0, \forall x, \forall y, \forall t\), for both simulation tests. When simulating the creep test, \(\sigma_{22} = f, \forall x, \forall y, \forall t\).
The distributions of displacement, \( u \) and \( v \), are linear functions of one space direction and independent from the second space direction, i.e.
\[
    u(x, y, t) = \epsilon_{11}(t) \frac{x}{l} \quad \text{and} \quad v(x, y, t) = \epsilon_{22}(t) \frac{y}{L}.
\]  \( \text{Eq. 13} \)

When simulating the relaxation test, \( \epsilon_{22}(t) = \delta L, \forall t \). We confront the numerical results with experimental data obtained on biological tissue. We use the results from [3] which were obtained from relaxation and creep tests done on samples of smooth muscle extracted from the soles of gastropods foots. The gastropods samples were tested by unidirectional loading on tensile apparatus. Relaxation tests were done on unfixed samples using the apparatus DMA 7 (dynamic mechanical analyzer, Perkin Elmer INC, Wellesley, Massachusetts) while creep tests were done on formalin-fixed samples using the apparatus Zwick/Roell SC-FR050TH (Zwick GmbH & Co., Ulm, Germany). The geometry of the tested samples and the values of loading are given in the table 3. The results of the experiments are plotted in fig. 3 and fig. 4 in term of elongation vs time for the creep test (fig. 3, solid curve), and in term of stress vs time for the relaxation test (fig. 4, solid curve). Then, numerical curves the best reproducing the experimental ones could be identified using the least-squares method. Identified values of the model parameters are given in tab. 3. The numerical simulations also give information on the horizontal deformation of the sample, \( \epsilon_{11} \), that was not stocked by the experimental measurements. Its (numerical) time evolution is plotted in fig. 5 and fig. 6. Nevertheless, the limitation of exploitation of this result lies with the fact that final solution strongly depends on the initial solution \( \epsilon_{11}^{\text{init}} \).

During the creep test the elongation of the gastropod sample increases in time, see fig. 3. Since this increase is not linear, the Maxwell model is not well suited. Indeed, the solutions \( b \) and \( p \) (= \( \dot{u}, \dot{v} \)) of the Maxwell model are stationary. Their analytical expressions are found when simulating the creep test:
\[
    \dot{\epsilon}_{11} = -\frac{\kappa f}{\eta}, \quad \dot{\epsilon}_{22} = \frac{f}{\eta}, \quad \forall x, \forall y, \forall t, \quad (MX \text{ model, creep test}).
\]  \( \text{Eq. 14} \)

On the other hand, the gastropod tissue shows stress relaxation: When simulating the relaxation test, stress decreases in time as shown in fig. 4. Even if the stationary solution is not reached within the tested interval of time, it seems that the stress does not decrease until it vanishes. Once more, the Maxwell model fails to mimic the gastropod tissue behaviour. Indeed, when simulating the relaxation test, the solutions \( \sigma_{22} \) and \( \dot{\epsilon}_{11} \) of the Maxwell model decrease till
vanishing. Moreover, if the compressibility coefficient is the same for the elastic and viscous elements, i.e. if $\nu = \kappa$, then the horizontal deformation is also stationary i.e. $\dot{\epsilon}_{11} = 0$, $\forall x$, $\forall y$, $\forall t$, see fig. 6.

For both kinds of loading, the solutions for the Kelvin-Voigt and the Three-Elements models have a tendency towards stationary values that are given in tab. 4. If the elastic elements of the Three-Elements model are identical, i.e. if $\nu_A = \nu_B \equiv \nu_{TE}$ and $E_A = E_B \equiv E_{TE}$, 

and if the conditions

$$E^{KV} = E^{TE}/2$$ and $$\nu^{KV} = \nu^{TE},$$

are fulfilled, then the stationary solutions are the same for both models. Moreover, when simulating the creep test, the following ways to reach the stationary solution are the same for both models if the condition $\eta^{KV} = \eta^{TE}/2$ are held. Then the creep solutions of the Kelvin-Voigt and the Three-Elements models become confused, see fig. 3 and fig. 5. On the other hand, the solutions diverge when simulating relaxation test, see fig. 4 and fig. 6. Here, all numerical simulations were done assuming the material to be compressible, with the same compressibility coefficient for all viscous or elastic elements: we fix $\kappa, \nu, \nu_A, \nu_B$ equals to 0.33 for each model.
Fig. 3. Creep test, confrontation between the three models and the experimental data.

Fig. 4. Relaxation test, confrontation between the three models and the experimental data.

Fig. 5. Creep test, evolution on the deformation $\epsilon_{11}$ for the three viscoelastic models.

Fig. 6. Relaxation test, evolution on the deformation $\epsilon_{11}$ for the three viscoelastic models.

and each simulation. Such assumptions forbid the Kelvin-Voigt model to relax. Indeed, the behaviour law (5) leads to the initial stress expression

$$\sigma_{22}^{\text{init}} = \frac{E}{1 - \nu^2} \left( \frac{\delta}{L} (1 - \nu \kappa) + \epsilon_{11}^{\text{init}} (\nu - \kappa) \right)$$

(KV model, relaxation test). (17)

(We recall that for the Kelvin-Voigt model, $\sigma_{22}^{\text{init}}$ is not a free model parameter but it is fixed by the constitutive equation since the later is not a differential equation for $\sigma$). This solution is confused with the stationary solution $\sigma_{22}^{\infty}$ (tab. 4) if $\nu = \kappa$. If not, the Kelvin-Voigt model relaxes, and by this way fundamentally diverges from its one-dimensional representation, which never relaxes. Also (for any compressibility coefficient) if the initial deformation $\epsilon_{11}^{\text{init}}$ is chosen equal to the stationary solution, $\epsilon_{11}^{\infty}$, then the Kelvin-Voigt model does not relax any more. On the other hand, the Three-Elements model relaxes whatever the initial value of the horizontal
deformation $\epsilon_{11}^{\text{init}}$ (assuming the (user free) initial value of the vertical stress, $\sigma_{22}^{\text{init}}$, chosen is different from the stationary one).

6. Conclusions

The two-dimensional extension of the classical linear viscoelastic models leads to systems of differential equations that are not solvable analytically. In general cases, stationary solutions can be found analytically but no analytical expression for the way to reach them can be provided. To study the mechanical behaviour of viscoelastic materials during mechanical loading we recourse to numerical solutions. In this contribution, we worked with the software Comsol Multiphysics. The mechanical equations are rewritten to be compatible with the predefined Comsol’s equations system, leading to a large amount of work on coefficients’ tensors identification which was done and is further developed in [4]. In this paper, we focus more on the results of the simulations. Numerical results were confronted with experimental data obtained on a sample of smooth muscle extracted from a gastropod intestine [3]. We conclude that the Maxwell model is unable to mimic the mechanical behaviour of such tissue, while the Kelvin-Voigt and the Three-Elements models leads to better results. We also observed that, excepting particular situations, the two-dimensional extension of the Kelvin-Voigt model relaxes and by this way fundamentally diverges from its one-dimensional representation, which never relaxes. We may finish by saying that all results are extremely sensible on initial solution which is not modeled by the rheological models but remain the user’s decision.

Acknowledgements

This work has been supported the Czech Ministry of Education, Sports and Youth, Project No. MSM4977751303., and by the French region Île-de-France by supporting the training period of N. Letzelter.

References