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Modelling the Mechanics of Timber Cell Walls

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ABSTRACT

Timber is a highly complex naturally occurring material, with properties adapted to its local environment. These properties, on its many length scales, determine its strength and stiffness and also how it interacts with moisture in the environment, causing dimensional instability both during drying and the lifetime of any building. Of particular importance is how the cell wall polymers interact with moisture in the environment and how this effects the properties, due to their strong dependence on intra-molecular hydrogen bonds. To model the dimensional behaviour of a wood cell under varying moisture conditions, the cell wall polymer matrix is modelled using a formulation of coupled deformation and moisture transport. These governing equations of mass and linear momentum conservation are strongly coupled and nonlinear and solved using the Finite Element Method. The associated constitutive equations are complex. The free energy is described through the deformation of the polymer matrix and the mixing with solvent (in this case, water). It is assumed that the polymer chains and water molecules are incompressible so that a change in volume of the polymer matrix corresponds to a change in the number of solvent molecules. The viscoelastic behaviour is resolved using a Zener spring-dashpot model, capturing both creep and relaxation phenomena, and the moisture transport is resolved using Fick's 2nd Law. The effects of wetting upon the stiffness and relaxation characteristics of the polymer matrix is taken into account through the chemical kinetics of hydrogen bond dissociation. Proper linearisation is achieved with automatic differentiation, using the library ADOL-C integrated with the group's FE code MOFEM.

Key Words: *Timber; Viscoelasticity; Finite Element Method; Coupled Problem*

1. Introduction

Timber is a highly complex multi-scale material, with properties of its many length scales. It is naturally occurring, with properties adapted to its local environment during growth, making timber an unpredictable material to work with. One particular problem is its dimensional instability when exposed to different environmental conditions, potentially causing issues during construction and the lifetime of a building. To enable prediction of dimensional changes in timber due to moisture sorption, the cell wall polymer matrix is modelled hygro-mechanically and the individual polymers are described chemically through the kinetics of hydrogen bond dissociation.

2. Timber Cell Wall

The wood cell wall is a multilayer composite structure, containing a primary cell wall and a 3 layer secondary cell wall. In the secondary cell wall, crystalline cellulose chains are arranged in a helical spiral. The chains are embedded within a polymer matrix consisting of amorphous cellulose, hemicelluloses and lignins. These polymers interact strongly with water, which binds to the hydroxyl groups contained within. This uptake of bound water within the cell wall replaces strong, intramolecular hydrogen bonds, leading to a corresponding loss of stiffness. Using an approach presented by Nissan [1], the Young's modulus of cellulose, at low moisture contents, can be related to the change in the number of intramolecular hydrogen bonds assuming each water molecule breaks one hydrogen bond. Considering the molecular weight of cellulose and water this yields:

$$\ln(N/N_0) = -1/3(w/W) \tag{1}$$

where N, denotes the number of effective hydrogen bonds at moisture content w, N_0 is the initial number of effective hydrogen bonds in the dry state, and W is the moisture content at which all hydroxyl groups carry one water molecule, which is close to 1/3 for cellulose. The number of hydrogen bonds can be related to the Young's modulus, E, as follows:

$$N = (E/k)^{1/3} \tag{2}$$

where the proportianality coefficient, k, describes the average force constant between the hydrogen bonds. By combining the equations we can formulate the change in Young's modulus, E/E_0, for low moisture contents,

$$\ln(E/E_0) = -w \tag{3}$$

where E_0 is the initial Young's modulus in the dry state. As the shear modulus is also dependent on the number of effective hydrogen bonds, the relationship can be adapted to incorportate shear modulus, G. The water content of each available sorption site can be described through the ratio of the number of moles of water and cellulose, and thus the mixture can be descibed in terms of its chemical potential, μ. By enforcing chemical equilibrium with the external environment, the conditions are present for diffusion to occur.

3. Model

Taking a similar approach to models on poroelastic gels [2], the cell wall polymer behaviour is modelled using a formulation of coupled deformation and moisture transport, described through linear momentum conservation Eq.(4) and the conservation of mass Eq.(5).

$$\mathrm{div}(\boldsymbol{\sigma}) = \boldsymbol{b} \tag{4}$$

$$\frac{\partial \varepsilon_{kk}}{\partial t} = -\frac{\kappa}{\eta\Omega}\mu_{,kk} \tag{5}$$

The volume change, $\varepsilon_{kk} = \Omega(C - C_0)$, where C is the concentration, assumes that the change of volume in the polymer network is due to the change in the number of bound water molecules. The volume of each water molecule, Ω, is constant, κ is the permeability and η is the viscosity of the polymer network. The moisture flux is given as $J_k = \mu_{,k}$.

The model is constitutively described using a Zener spring-dashpot configuration, shown in Figure 1. This arrangement allows both creep and relaxation phenomena to be captured. The model is formulated in terms of its external state variables (ε, σ) and (C, μ), representing the mechanical and chemical behaviour respectively, and the internal state variable, $\hat{\varepsilon}$, which represents the internal rearrangement of intramolecular hydrogen bonds under stress.

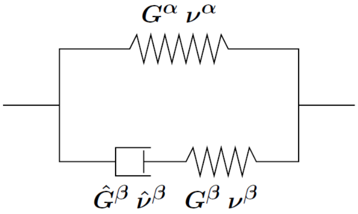

Figure 1: : Model representing a rheological Zener spring-dashpot arrangement. The spring α represents the instantaneous elasticity of the polymer network. The spring and dashpot in series arrangement, β, represents the viscoelastic relaxation.

The stress, σ, within the system Eq.(7) can be specified as the the sum of the stress within spring α, spring β and the hydrostatic pressure due to the concentration of solvent molecules, $\hat{\sigma}^{\beta}$, Eq.(6).

$$\hat{\sigma}^{\beta} = \frac{\Delta\mu}{\Omega}\,\mathrm{I} \tag{6}$$

$$\sigma = \sigma^{\alpha} + \sigma^{\beta} - \hat{\sigma}^{\beta} \tag{7}$$

The stresses within the individual springs, α and β, are specified in Eq.(8) and (9), where G^{α} and G^{β} are the shear moduli of each spring respectively and ν^{α} and ν^{β} are the Poisson's ratios.

$$\sigma^{\alpha}_{ij} = 2G^{\alpha}\left[\varepsilon_{ij} + \frac{\nu^{\alpha}}{1-2\nu^{\alpha}}\,\varepsilon_{kk}\,\delta_{ij}\right] \tag{8}$$

$$\sigma^{\beta}_{ij} = 2G^{\beta}\left[(\varepsilon_{ij} - \hat{\varepsilon_{ij}}) + \frac{\nu^{\beta}}{1-2\nu^{\beta}}\,(\varepsilon_{kk} - \hat{\varepsilon}_{kk})\,\delta_{ij}\right] \tag{9}$$

When stress is applied to the system, the viscous motion of the dashpot determines the rate at which spring β relaxes, Eq.(10). The viscous behaviour is determined by the rate of breakdown of intromolecular hydrogen bonds within the network, $\hat{G}^{\beta}$, and Poisson's ratio $\hat{\nu}^{\beta}$, which controls the time dependent deformation.

$$\frac{\partial\hat{\varepsilon_{ij}}}{\partial t} = \frac{1}{2\hat{G}^{\beta}}\left[\sigma^{\beta}_{ij} - \frac{\hat{\nu}^{\beta}}{1+\hat{\nu}^{\beta}}\,\sigma^{\beta}_{kk}\,\delta_{ij}\right] \tag{10}$$

4. Finite Element Implementation

The model is formulated in 3D using the Finite Element Method using MOFEM. The mesh consists of 10 node tetrahedral elements with a higher order of approximation applied to the displacement field to allow for the different orders of the two governing equations (Eq. (4) and (5)), ensuring stability. The tangent matrices are calculated using automatic differentiation (ADOL-C) to achieve proper linearisation.

$$\left(f_x{}^{internal}\right)_i = \int_V \frac{\partial N_i}{\partial X_j}\,\sigma_{ij}\,dV \tag{11}$$

$$\left(f_{\mu}{}^{v}\right)_j + \left(f_{\mu}{}^{J}\right)_j = \int_V N_j\,\frac{\partial V}{\partial t}\,dV + \int_V \frac{\partial N_j}{\partial X_k}\,J_k\,dV \tag{12}$$

$$(r_{\hat{\varepsilon}})_j = \int_V N_j\left(\frac{\partial\hat{\varepsilon}}{\partial X_j} - f(\sigma^{\beta})\right)dV \tag{13}$$

Equations (11) - (13) represent the internal force, the flux and the residual strain respectively, where N is a matrix of shape functions , $f(\boldsymbol{\sigma})$ is a function for a linear viscous material, and the volume is given by V. They are assembled in the system as follows:

$$\begin{bmatrix} K_{xx} & K_{x\mu} & K_{x\hat{\varepsilon}} \\ K_{\mu x} & K_{\mu\mu} & K_{\mu\hat{\varepsilon}} \\ K_{\hat{\varepsilon}x} & K_{\hat{\varepsilon}\mu} & K_{\hat{\varepsilon}\hat{\varepsilon}} \end{bmatrix} \begin{bmatrix} q_x \\ q_{\mu} \\ q_{\hat{\varepsilon}} \end{bmatrix} = \begin{bmatrix} f_x{}^{external} - f_x{}^{internal} \\ f_{\mu}{}^{v} + f_{\mu}{}^{J} \\ r_{\hat{\varepsilon}} \end{bmatrix}$$

The polymer network is described in terms of a rectangle, enforcing symmetry on the y axis, shown in figure 2. The Boundary condition μ, representing the external moisture conditions, is applied on all faces and held constant, with the exception of the symmetrical face where the flux is set to zero. A tensile force is applied in the y-direction and released once equilibrium has been reached.

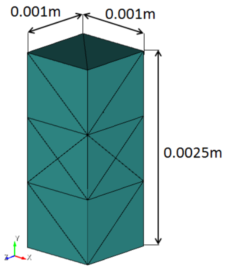

Figure 2: : Rectangular bar mesh consisting of 10 node tetrahedral elements, representing a 1/4 sample with symmetry on the x,y and z axis.

5. Numerical Example

A specimen, Figure 2, is loaded in tension. The load is held for 35 minutes and then released. The creep results shown in Figure 3 (right) demonstrate the coupling between the mechanical and hygral behaviour. The graph shows the displacement of the top face vs the chemical potential at the mid point of the specimen. Initially the applied force causes an elastic displacement, elongating the sample and causing a dip in the chemical load in the middle of the sample. The evolution of the chemical load through the sample is shown in Figure 3 (left). Over a longer length of time the sample then undergoes creep, increasing the displacement until it reaches equilibrium. At this point all the stress is taken by spring α. The load is then released, causing an increase in chemical load which reduces over time as the sample returns to its reference configuration.

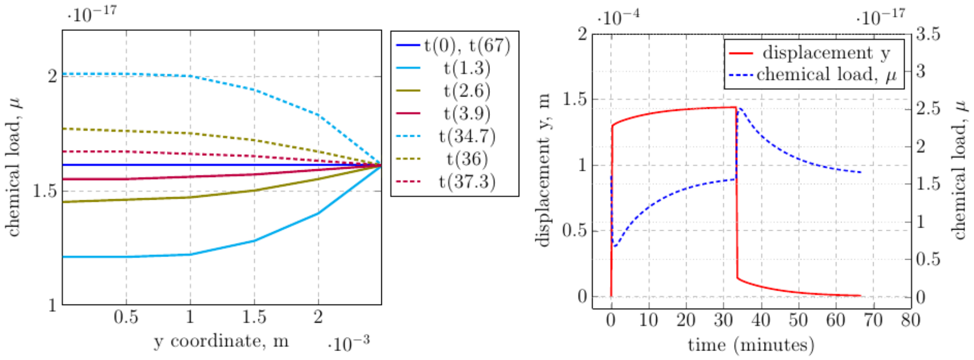

Figure 3: : Left: Evolution of the chemical load through the sample along the y-axis at given time steps, t(min), where the solid lines occur during the loading phase and the dashed lines occur post loading. Right: Demonstration of the coupling between the chemical load and the displacement due to an external force applied to the sample

6. Conclusions

The proposed model is currently formulated in small strains and as such can only be applied to small changes in deformation and cannot yet fully describe the mechano-soprtive behaviour in environmental conditions that exceed 50% relative humidity. All viscoelastic changes are fully reversible, and after a short time the sample with return its reference configuration if the conditions return to those at time zero. In the future the model will be formulated in large strains and take into account a larger degree of polymer softening at higher moisture contents.

References

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