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Modeling the hygroexpansion of aligned wood fiber composites

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ABSTRACT

The effect of wood fiber ultrastructure and cell wall hygroelastic properties on wood fiber composite hygroexpansion has been analyzed. An analytical concentric cylinder model extended to include also free hygroexpansion of orthotropic phase materials has been used on several length scales. Using properties of the three main wood polymers, cellulose, hemicellulose and lignin the longitudinal and transverse hygroexpansion coefficients for the microfibril unit cell were obtained and the volume fraction change of the wood polymers in the microfibril unit cell depending on relative humidity was calculated. The fiber cell wall was modeled regarding each individual S1, S2 and S3 layer and the cell wall longitudinal hygroexpansion coefficient was determined depending on microfibril angle in the S2 layer. A homogenization procedure replacing the S1, S2 and S3 layers with one single layer was found not to influence the results significantly for low microfibril angles. Finally the hygroexpansion coefficients of an aligned softwood fiber composite were calculated.

1. Introduction

Wood and other lignocellulosic fiber reinforced polymers have large potential as structural materials due to the high specific stiffness, high specific strength and high aspect ratio of the fibers [1]. Still their broad application is limited by some major disadvantages and the fibers susceptibility to moisture uptake is one of them. Cellulosic fiber composites tend to swell considerably at water uptake and as a consequence mechanical properties, such as stiffness and strength, are negatively influenced [2]. The fiber swelling may be reduced by means of chemical, enzymatic or mechanical modifications [3]. Nevertheless, the swelling mechanisms of cellulose fiber composites must be better understood if they are to reach their full potential.

At micron length-scale the softwood fiber cell (tracheid) consists of several layers surrounding the lumen with the outermost layer being the primary wall (P) preceded by the outer layer of the secondary wall (S1), the middle layer of the secondary wall (S2) and the inner layer of the secondary wall (S3). At an ultrastructural level the layer structure resembles that of a fiber reinforced composite, the reinforcing element being the cellulose microfibril units embedded in a matrix of the wood polymers lignin and hemicelluloses [4]. The cellulose microfibrils are aligned fairly parallel in a helical pattern within each layer. The microfibril angle (MFA) in a layer is the angular deviation of the microfibrils from longitudinal fiber axis. The macro-properties of a wood fiber composite is governed by the properties of its constituents fiber and matrix, their relative volume fractions, interface properties and by microarchitecture, i.e. the fiber orientation distribution, fiber shape, lumen size and whether the lumen is filled with resin or not.

The link between ultrastructure to mechanical behavior and hygroelastic properties of wood fibers have been studied by several authors [5–14]. Barber et al. [5,6] used laminate theory to model the anisotropic shrinkage of wood in connection with variation of MFA in the S2 layer. Later Barber [6] modified the model representing the wood cell as a thick-walled cylinder to investigate the effect of layers and validate the simplifying assumption made in [5] that the cell wall may be treated as a flat surface. Koponen et al. [8] represented a unit of two adjacent cell walls as a balanced and symmetric laminate and layer properties were modeled from an ultrastructural level with moisture dependent elastic properties based on values by Cousins and Cave [15–17]. A similar approach was used also by Thuvander et al. [9] to model the cell wall drying stresses in wood. A rather comprehensive numerical modeling work of wood was made by Persson [10]. Neagu and Gamstedt [14] modeled the hygroexpansion of a typical softwood fiber based on a state space approach. The wood fiber was modeled as an assembly of coaxial hollow cylinders made of orthotropic material of helical structure.

The objective of this paper is to analyze the effect of constituent hygroelastic properties on all length scales from ultrastructural properties to unidirectional (UD) composite properties. An analytical concentric cylinder (CC) model valid for orthotropic phase materials and for an arbitrary number of phases was developed previously by the authors [18]. The same CC-model will be used also in this work, adding hygroexpansion terms. First the material

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model will be outlined and then the hygroelastic properties on three scales will be calculated: (i) swelling characteristics on the ultrastructural level, i.e. the microfibril unit cell (UC) in layers S1, S2 and S3, (ii) the hygroexpansion coefficients of the fiber wall, (iii) the hygroexpansion coefficients of the aligned wood fiber composite. Aligned wood fiber composites are used in laminate analogy models to describe the behavior of wood fiber composites. A short-fiber composite with a certain fiber orientation distribution is replaced by a laminate with many thin UD layers [19]. The layer volume fractions reflect the fiber orientation distribution.

Assumptions regarding the fiber and its interaction with the matrix are: (i) The fiber may be seen as an assembly of long coaxial hollow cylinders with high aspect ratio meaning that the stress transfer zone extends only over a small part of the interface and perturbation effects related to fiber ends may be neglected. In reality the cross-sectional shape varies from being thick-walled box-like for most of the latewood fibers to a relatively slender rectangular form for the thin-walled earlywood fibers. (ii) The bonding between fiber and matrix is perfect and the fiber is free from defects, i.e. kinks, pits, etc. (iii) Since the fiber is embedded in the matrix the fiber rotation due to its helical structure is restricted. Furthermore, no bending of the fiber due to axial load is expected and thus the fiber wall performs as a balanced and symmetric laminate. These assumptions are rather crude and specific for fibers in composites, so the values presented herein must therefore be thought of as "in situ" fiber properties.

2. Theory

Moisture absorption leads to an increase in moisture weight content and dimensional changes of the fiber. These changes are assumed to be proportional to the moisture content change and for orthotropic materials three constant coefficients of proportionality called hygroexpansion coefficients are introduced

$$\beta_j^H = \frac{\varepsilon_j^H}{\Delta M} \quad j = 1,2,3 \tag{1}$$

Here ε_j^H is the free swelling strain in j- direction due to a moisture weight content change by ΔM. Composite materials contain multiple connected phases with different swelling coefficients and different moisture contents. The free (unconstrained) average swelling of the composite is the result of internal force balance and depends on the composite microstructure and the hygroelastic properties of its constituents. In the following section the moisture expansion analysis based on the concentric cylinder (CC) assembly model is presented. The model is valid for an arbitrary number of orthotropic phases/layers, and thus we are inherently neglecting the fiber tendency to rotate. As the result of phase swelling only normal stresses and strains develop. The difference with the model here compared to the CC-model previously presented by the authors in [18] is that free moisture expansion terms are added in the elastic stress–strain relationship

$$\sigma_i = C_{ij}(\varepsilon_j - \varepsilon_j^H) \tag{2}$$

C_{ij} is the stiffness matrix with usual notation. Performing the same derivations as in [18] the expressions for radial displacement, radial- and axial stress are modified, for more detail see Appendix. The expressions for the kth phase are now given by

$$u_r^k = A_1^k r^{\alpha_k} + A_2^k r^{-\alpha_k} + \psi_k \varepsilon_{10} r - H_k^* \Delta M_k r \tag{3}$$

$$\sigma_r^k = A_1^k \beta_k r^{\alpha_k - 1} + A_2^k \gamma_k r^{-\alpha_k - 1} + \varphi_k \varepsilon_{10} - H_r^k \Delta M_k \tag{4}$$

$$\sigma_1^k = A_1^k f_k r^{\alpha_k - 1} + A_2^k h_k r^{-\alpha_k - 1} + g_k \varepsilon_{10} - H_1^k \Delta M_k \tag{5}$$

r is the radial coordinate and ε_{10} the strain in direction 1 (axial). ΔM_k is the moisture weight content change in the kth phase used as input data. A_1^k and A_2^k are unknown constants yet to be found and α_k, ψ_k, β_k, γ_k, φ_k, g_k, f_k and h_k are functions of the kth phase elastic constants given by Eqs. (A5), (A8) and (A12) in Appendix. In Eqs. (3)–(5) we also have

$$H_k^* = \frac{1}{C_{22}^k - C_{33}^k}\left[(C_{13}^k - C_{12}^k)\beta_{1k}^H + (C_{23}^k - C_{22}^k)\beta_{rk}^H + (C_{33}^k - C_{23}^k)\beta_{\theta k}^H\right] \tag{6}$$

$$H_r^k = C_{12}^k \beta_{1k}^H + C_{22}^k \beta_{rk}^H + C_{23}^k \beta_{\theta k}^H + (C_{22}^k + C_{23}^k) H_k^* \tag{7}$$

$$H_1^k = C_{11}^k \beta_{1k}^H + C_{12}^k \beta_{rk}^H + C_{13}^k \beta_{\theta k}^H + (C_{12}^k + C_{13}^k) H_k^* \tag{8}$$

For isotropic or transversely isotropic materials $H^* = 0$. The displacement and stress expressions (3)–(5) have to satisfy continuity conditions on all interfaces:

(i) Radial displacement must be zero on the symmetry axis

$$u_r^1(r = 0) = 0 \tag{9}$$

(ii) Displacement and radial stress continuity conditions at all interfaces

$$u_r^k(r_k) = u_r^{k+1}(r_k) \quad k = 1,2,\ldots,N-1 \tag{10}$$

$$\sigma_r^k(r_k) = \sigma_r^{k+1}(r_k) \quad k = 1,2,\ldots,N-1 \tag{11}$$

(iii) Zero radial stress at the outer boundary $r = r_N$ of the cylinder assembly

$$\sigma_r^N(r_N) = 0 \tag{12}$$

The strain ε_{10} in direction 1 is constant and its value must result in zero average stress in direction 1 leading to

$$\sigma_1^{av} = \frac{2}{r_N^2}\sum_{k=1}^{N}\int_{r_{k-1}}^{r_k} r\sigma_1^k(r)\mathrm{d}r = 0 \tag{13}$$

Insertion of Eq. (5) in (13) and integration yields

$$\sum_{k=1}^{N}\left(\frac{A_1^k f_k}{\alpha_k + 1}(r_k^{\alpha_k+1} - r_{k-1}^{\alpha_k+1}) + \frac{A_2^k h_k}{-\alpha_k + 1}(r_k^{-\alpha_k+1} - r_{k-1}^{-\alpha_k+1}) + \frac{r_k^2 - r_{k-1}^2}{2}(\varepsilon_{10} g_k - H_1^k \Delta M_k)\right) = 0 \tag{14}$$

Some sub-cylinders in the assembly may be transverse isotropic or isotropic. For such sub-cylinders (phases) $\alpha_k = 1$, $h_k = 0$ and the second term in Eq. (14) is zero. The unknown constants A_1^k and A_2^k for $k = 1,\ldots,N$ can be determined by solving a system of linear algebraic equations using the displacement and stresses in Eqs. (3)–(5) in Eqs. (9)–(12). The problem is conveniently solved by using ε_{10} as a numerical parameter. The system is solved for every value of ε_{10} and Eq. (14) used to check whether average stress is zero. When ε_{10} is determined the hygroexpansion coefficients of the assembly may be calculated from

$$\beta_L^H = \frac{\varepsilon_{10}}{\Delta M_{avg}} \quad \beta_T^H = \frac{\varepsilon_r^{avg}}{\Delta M_{avg}} = \frac{u_r(r_N)}{r_N \Delta M_{avg}} \tag{15}$$

The expression for radial displacement u_r is given by Eq. (3). The average moisture content of the analyzed assembly ΔM_{avg} obeys the rule of mixtures

$$\Delta M_{avg} = \sum_k \Delta M_k \frac{\rho_k}{\rho_{avg}} V_k \tag{16}$$

$$\rho_{avg} = \sum_k \rho_k V_k \tag{17}$$

where ρ_k is the initial density and V_k the volume fraction of phase k, i.e. before swelling.