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Modelling longitudinal elastic an shrinkage properties of wood

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Summary. A model was developed for estimating elastic and shrinkage properties of a softwood cell wall from the properties of its polymeric constituents: cellulose, hemicellulose and lignin. The theory of composite materials was used. Based on a literature survey, models of latewood, earlywood and compressionwood of a softwood cell wall structure were made. The model takes into account the helical winding of the microfibrils in the cell wall and it estimates the behaviour of a balanced laminated double-cell wall in which rotation is restrained by adjacent cells. The calculated elastic and shrinkage properties were compared with earlier test results and good agreement was found.

Introduction

A model was developed for estimating elastic and shrinkage properties of a softwood cell wall from the properties of its polymeric constituents: cellulose, hemicellulose and lignin.

The elastic constants of the cell wall were calculated with equations derived by P.C. Chou, J. Carleone and C.M. Hsu (1972) in a 3-dimensional case, where the layered media was replaced by an equivalent homogeneous material. The assumptions made are from a combination of the Voigt's and Reuss' theory on composite materials. The mathematics involved are not presented here; for further reference see Koponen et al. (1987). The material is assumed to be ideal elastic and rotation or loss of stability of the cell is not considered.

Figure 1 shows four different levels of magnification of the wood material. Level I shows the annual rings of wood, level II shows a group of cells cut from a part of the annual ring, level III shows the cell wall cross-section and level IV one layer of the cell wall with inclined microfibrils embedded in a matrix. The model simulates the elastic an shrinkage properties on levels III and IV so far. The variables involved in this study are the inclination of microfibrils in the S2-1ayer, moisture content of wood and cell type (early, late- and compressionwood). The model will be extended to levels I and II to simulate the whole complex structure of wood.

Structural model of the cell wall

In this model the cell wall consists of layers $M + P$, S1, S2 and S3, and two adjacent cell walls are examined as a unit. The secondary wall consists of microfibrils embedded

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Fig. 2. Cross section of the microfibril

in lignin and the middle lamella consists of lignin only. The cross-section of the microfibril is assumed in the calculations to be as in Fig. 2. The volumetric portion of cellulose is 49%, hemicellulose 24% and lignin 27%.

The elastic constants for cellulose are:

$$
C_s = \begin{bmatrix} 137 & 14 & 14 & 0 & 0 & 0 \\ 14 & 27.2 & 14 & 0 & 0 & 0 \\ 14 & 14 & 27.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.4 \end{bmatrix} \cdot 10^9 \text{ Pa}
$$

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These values were obtained from earlier works of Sakurada et al. (1962) and Mark (1967). The longitudinal elastic modulus was evaluated experimentally and the others by theoretical calculations. Cellulose is assumed not to react with moisture in any way.

Lignin is an isotropic material and its elastic constants are:

$$
C_1 = \begin{bmatrix} 4 & 2 & 2 & 0 & 0 & 0 \\ 2 & 4 & 2 & 0 & 0 & 0 \\ 2 & 2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot c(u)_{iig} \cdot 10^9 \text{ Pa}
$$

These values were obtained from studies of Cousins (1976) and Cave (1978). The elastic constants of lignin change as a function of moisture content, as in Fig. 3, this is taken into account with the variable $c(u)_{\text{liq}}$ which has a maximum value of 1.75 at 4% moisture content.

Lignin is assumed to shrink corresponding to the volume of released moisture.

$$
\epsilon_i^o = \{1, 1, 1, 0, 0, 0\} \cdot \Delta V / 3, (i = 1, 2, \dots, 6)
$$

where ΔV is amount of released moisture.

The elastic constants of hemicellulose are:

2 4 2 0 0 0 t 2 2 0 0 i] Ch = 2 2 4 0 0 0 .C(U)hem.109Pa 0 0 0 1 0 0 0 0 1 0 0 0 0

Moisture dependance of the elastic constants of hemicellulose is taken into account with the factor $c(u)_{hem}$. The longitudinal elastic modulus varies with moisture content according to Fig. 4. These values are based on studies of Cousins (1978) and Cave (1978).

Cave (1978) assumed that hemicellulose does not shrink in the longitudinal direction, since it is isotropic only in the cross direction. The shrinkage of hemicellulose is given as:

$$
\varepsilon_i^o = \{0, 1, 1, 0, 0, 0\} \cdot \Delta V / 2 \ (i = 1, 2, \dots, 6)
$$

The structure of the cell wall for late-, early- and compression wood is given in Table 1. The volumetric portions and microfibril angels in each cell wall layer are presented.

The cell wall layer \$3 is divided into three equal parts having microfibril angles of -45° , 45° and 90°. The layer S1 is divided into two equal parts having microfibril angles of -80° and 80° . In the calculations the microfibril angle of S2 layer varies $0^\circ - 30^\circ$ in latewood, $10^\circ - 40^\circ$ in earlywood and $30^\circ - 70^\circ$ in compressionwood. It is assumed that the cell wall remains as a plane at all times and no twisting or loss of stability will take place.

Fig. 3. Dependence of the stiffness moduli C_{11} of lignin on moisture content

Fig. 4. Dependence of the longitudinal stiffness moduli C_{11} of lignin on moisture content

Table 1. Volumetric proportions of cellulose, hemicellulose and lignin in the cell wall used used in calculations

Cell type	Cellulose $V - \frac{9}{6}$	Hemicellulose $V - \frac{6}{6}$	Lignin V ⁰ / ₀
Latewood	46	22	32
Earlywood	40	20	40
Compressionwood	45	23	32

Calculated elastic and shrinkage properties of the cell wall

The stiffness matrix and the shrinkage of the cell wall was calculated by a computer program. It was assumed that the cell wall is in an unstressed state at saturation point.

Figure 5 presents the calculated longitudinal elastic modulus of the cell wall of late-, early- and compressionwood as a function of the microfibril angle of the \$2 layer at different moisture contents. In latewood the elastic modulus of the cell wall varies 35-58 GPa at microbfibril angles of 0° -20°. The effect of moisture is 5-10% to the elastic modulus. In earlywood the elastic modulus of the cell wall varies 8-39 GPa (microfibril angles $15^{\circ} - 40^{\circ}$). The effect of moisture is bigger than in latewood, 10-20%. In compressionwood the elastic modulus varies $1-20$ GPa $(30^{\circ} - 60^{\circ})$ and the effect of moisture can be over 50% at the bigger microfibril angles.

From these results the longitudinal elastic modulus of wood can be estimated. For example the density of the cell wall is 1500 kg/m^3 , and we assume the density of

Fig. 5. Calculated longitudinal elastic modulus of the cell wall at different microfibril angles and moisture contents

Layer	V_{\cdot} %	θ degree
Latewood:		
S3	2.0	$-45, +45, 90$
S2	80.0	$0 - 30$
S ₁	4.0	$-80, +80$
$P + M$	7.0	lignin
Earlywood:		
S3	5.0	$-45, +45, 90$
S2	67.5	$10 - 40$
S ₁	10.0	$-80, +80$
$P + M$	17.5	lignin
Compressionwood:		
S3	missing	
S ₂	83.3	$30 - 70$
S ₁	8.3	$-80, +80$
$P+M$	8.4	lignin

Table 2. Structure of the cell wall for cell types used in the model

earlywood to be 340 kg/m³ and the microfibril angle of the S2 layer 30 \degree , the porosity of earlywood will be 0.773 and the elastic modulus varies 18-21 GPa depending on moisture content. Taking into account the porosity we get an elastic modulus of 4.1-4.6 GPa for earlywood. For latewood the density is 860 kg/m^3 and the microfibril angle of the $S2$ layer 10° . The porosity of latewood is 0.427 and we get an elastic modulus of 29-31 GPa. If we have a wood of 480 kg/m³ density, it would be 73% earlywood and 27% latewood and if the shrinkage of the cross-section area is taken into account (for softwoods it is about 11%) elastic modulus would be $9.8-12$ GPa depending on moisture content. From literature a softwood of density 480 kg/m^3 would have an elastic modulus of 11.8 GPa. The calculations match very well.

The other elastic constants are not presented here. The whole stiffness matrix is presented in Koponen et al. (1987).

In calculating the shrinkage, the cell wall is dried from the saturation point $(u = 30\%)$ to completely dry $(u = 0\%)$. The drying of the cell wall is calculated in 20 steps. At the saturation point the cell wall is assumed to be in an unstressed state. No creep factors have been taken into account.

Figure 6 shows the calculated shrinkage of latewood in the longitudinal direction and Fig. 7 the experimental shrinkage of latewood of some species tested by Koehler (1931). In Fig. 6, 10 to 13 shrinkage is stated by a negative sign and swelling by a positive sign. According to the model latewoods longitudinal dimension increases as it dries, when the microfibril angle of $S2$ layer is greater than 10° . Experimental results also support this phenomenon. The experimental shrinkage curves match with the shrinkage curves of the model at microfibril angles of $0^\circ - 20^\circ$.

Figures 8 and 9 present the calculated and experimental shrinkages for earlywood and Figs. 10 and 11 the corresponding results for compressionwood. The calculated shrinkages of earlywood match with the experimental results at microfibril angles of 10° – 40° and the shrinkages of compressionwood at a microfibril angle of about 50°.

Fig. 6. Calculated longitudinal shrinkage of latewood

Fig. 7. Experimental shrinkage of latewood for different species (Koehler 1931). 1, 2 = *Pinus echinata; 3 = Sequoia sempervirens; 4 = Pseudotsuga taxifolia*

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Fig. 8. Calculated longitudinal shrinkage of earlywood

Fig. 9. Experimental shrinkage of earlywood for different species (Koehler 1931). 1 = *Pinus eehinata; 2 = Pseudotsuga taxifolia; 3 = Sequoia sempervirens*

Fig. 10. Calculated longitudinal shrinkage of compressionwood

Fig. 11. The experimental longitudinal shrinkage of the compressionwood 0f ponderosa pine (Koehler 1931)

Fig. 12. The calculated final longitudinal shrinkage of latewood (L) , earlywood (E) and compressionwood (C) at different microfibril angles

Fig. 13. Experimentally determined final longitudinal and tangential shrinkage at different microfibril angles (Meylan 1972)

The calculated final shrinkages when the cell wall is completely dried are presented in Fig. 12 as a function of the microfibril angle. The shrinking of latewood turns to length increase when the microfibril angle is over 10° . In earlywood length increases at microfibril angles of $25^\circ - 35^\circ$. Shrinking increases dramatically at microfibril angles $35^\circ - 60^\circ$. B. A. Meylan (1972) has determined the effect of the microfibril angle of the S2 layer on the final shrinkages in the direction of the grain by testing small specimen of *Pinus jeffreyi.* Most of the specimen were earlywood. These test results, Fig. 13, show a very similar shrinkage curve as the ones determined theoretically.

The shrinkages of the cell wall in the tangential and radial directions were also determined. These are not presented here, for reference see Koponen et al. (1987). These values cannot be compared directly to the shrinking of wood in the cross directions, since the cellular structure of wood (Levels I and II of Fig. 1) should be taken into account.

Conclusion

The parameters used in modelling the cell wall are based on a literature survey. Some of these values were determined experimentally, some of them were evaluated theoretically and some are assumptions based on other materials. Although some of these parameters are uncertain, the model gave encouraging results. In modelling the cell wall the most important structural parameters are the quantities and distribution of Modelling properties of wood 63

cellulose, hemicellulose and lignin in the different cell wall layers, the microfibril angles in the different cell wall layers and the cell wall layer widths. The most important material parameters are the elastic constants and the shrinkage properties of cellulose, hemicellulose and lignin. These parameters have yet different weights depending on what property is being calculated. For example in calculating the longitudinal elastic modulus of the cell wall special emphasis must be given to the longitudinal elastic modulus of cellulose, cellulose content, width of the \$2 layer and its microfibril angle. In calculating other elastic constants and shrinkages, equal emphasis should be given to all the cell wall layers.

The results calculated with this model are in good agreement with earlier test results. The elastic modulus of the cell wall and its dependence on the microfibril angle of the \$2 layer match well with the results of other authors. Also the known different shrinkage properties of late-, early- and compressionwood can be explained with this model.

The model will be extended to cover a group of cells and moreover the annual ring formation of wood to simulate elastic and shrinkage properties both in longitudinal and in parallel directions.

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