From clear soft wood to reaction wood : modeling of the influences of the microfibril angle and specific gravity on mechanical properties, elasticity and shrinkage

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Abstract

A predictive mechanical modelling, based on a micro-macro approach, integrating four successive levels (macromolecules - cell wall - ligneous tissues - annual ring) and using 29 parameters of the structure and the ultra structure, allows to calculate three elastic modulus E_R, E_T and E_L of clear wood. A particular set of those parameters characterises the standard softwood.(see SWW column A on table 1).
The purpose of this paper is to illustrate the utilisation of this mechanical model to analyse the influence of structural and ultra structural changes in reaction wood, according to bibliography, and to discuss the consequences on the macroscopic elastic properties of compression wood.

1. INTRODUCTION

It is now well known that the specific gravity, the moisture content and eventually the temperature are physical parameters governing the mechanical properties of woods, in particular the elastic anisotropy. Predictive models were proposed [1] for clear softwoods to characterise the three young modulus E_R , E_T and E_L, respectively, along the radial, tangential and longitudinal anatomical directions as a linear functions of the specific gravity ρ.
That is to say that the observed variability of elastic properties of different normal woods is well explained by those parameters.
The paradox is that the variability of elastic properties inside a given tree can be significantly larger and the specific gravity, the moisture content and the temperature are no more pertinent parameters. This variability, inside the tree, is governed by more complex anatomical parameters that characterise the different woods, juvenile wood, adult normal wood, compression wood,…
The purpose of this paper is to illustrate and analyse the influence of small realistic variations of structural and ultra structural parameters on the macroscopic elastic anisotropy of softwood, to characterise more specifically the transition from normal wood to reaction wood.

2. PRINCIPLE OF THE MECHANICAL MODELLING AND PROPERTIES OF THE STANDARD SOFTWOOD (SSW)

A predictive mechanical modelling, based on a micro-macro approach, integrating four successive levels and using 29 parameters of the structure and the ultrastructure, allows to calculate three elastic modulus E_R , E_T and E_L of a given clear wood [2]. The modelling presented previously [2], [3] should not be discussed here.

2.1. Step 1-2 : Cell wall elastic properties

The two first steps of the mechanical modelling (here combined in a single step [1]) give an estimation of the longitudinal E_{Lp} (1) and transverse E_{Tp} (2) Young modulus of the double cell wall belonging to two adjacent wood cells, which is assimilated to an isotropic matrix of amorphous hemicellulose and lignin reinforced by a three dimensional skeleton of crystalline cellulose microfibrils. Note that the model considers mainly the S_2 sub layer, influences of S_1 and S_3 are neglected .

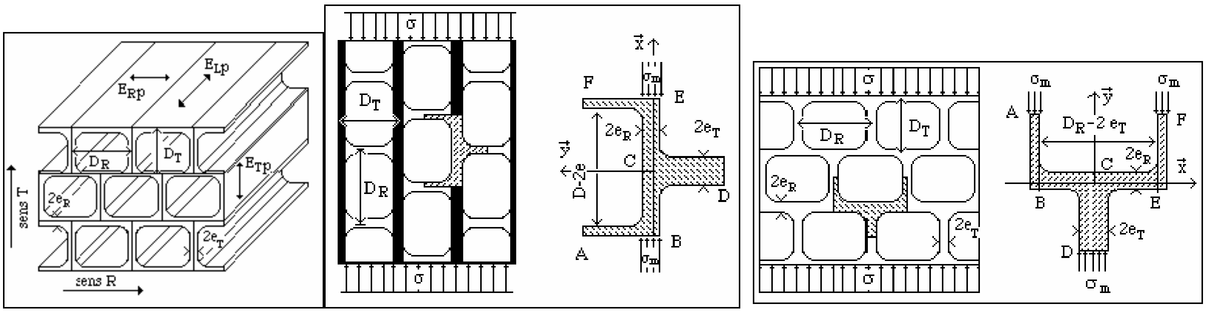

Figure 1 : Geometric parameters of the honeycomb of rectangular cells

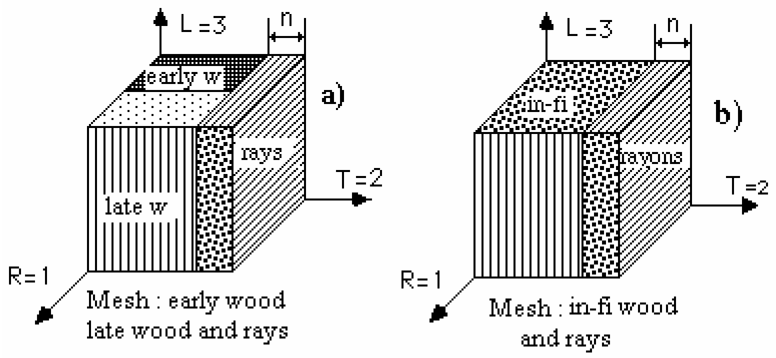

Figure 2 : Mesh of an annual ring : a) three tissues early wood, late wood and rays
b) after homogenisation of early wood and late wood in in-fi wood.

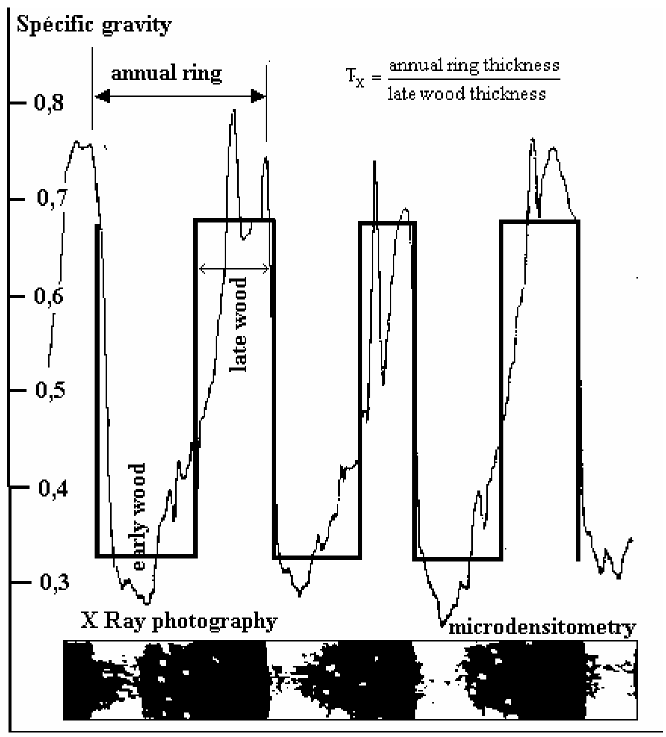

Figure 3 : Evolution of specific gravity inside annual rings through a microdensitometry Xray photograph .
Approximation of the heterogeneity inside the annual ring through the texture T_x

The five input parameters are the Young modulus E^m and the Poisson ratio ν^m of the isotropic matrix, the Young modulus E^f, the volume ratio V and φ the microfibril angle (MFA).

$$E_{Lp} = (1-V)\frac{(1-\upsilon^m)}{(1+\upsilon^m)(1-2\upsilon^m)}E^m + V(1-\sin^4(\varphi))E^f \qquad (1)$$

$$E_{Tp} = E_{Rp} = (1-V)\frac{(1-\upsilon^m)}{(1+\upsilon^m)(1-2\upsilon^m)}E^m + V(1-\cos^4(\varphi))E^f \qquad (2)$$

2.2 Step 3 : ligneous tissues elastic properties

The third step of the mechanical modelling gives the longitudinal E_L^x and transverse E_T^x Young modulus of a ligneous tissue (x) assimilated to a honeycomb of rectangular cells, whose cell walls are in file along the radial direction R and alternated along the tangential direction T (figure 1)
The four new ininput geometric parameters are the diameters D_R and D_T and the thickness e_R and e_T of the rectangular tissue cell, respectively along radial and tangential directions.

$$E_L^x = 2\left[\frac{e_T}{D_R} + \frac{e_R}{D_T} - 2\frac{e_T e_R}{D_R D_T}\right]E_{LP} \qquad (3)$$

$$\frac{1}{E_T^x} = \left[1 + \frac{1}{16}\frac{E_{TP}}{E_{RP}}\frac{e_T}{D_T}\frac{(D_R - 2e_T)^3}{e_R^3}\right]\frac{D_R}{2e_T}\frac{1}{E_{TP}} \qquad (4)$$

We must notice that assuming, as usually, that the specific gravity of the cell wall material is a constant (ρ_p = 1,51 g.cm^{-3}) then the specific gravity of the considered wooden tissue ρ^x is directly connected to the geometric parameters.

$$\rho^x = (1-P_0)\,\rho_P = 2\left[\frac{e_T}{D_R} + \frac{e_R}{D_T} - 2\frac{e_T e_R}{D_R D_T}\right]\rho_P \qquad (5)$$

where P_0 is the porosity of the tissue.
As a consequence, for a given specific gravity ρ^x of the wooden tissue the geometric parameters are no more independent.

2.3 Step 4 : clear wood elastic properties

The fourth and last step of the mechanical modelling takes into account the heterogeneity of the annual ring. Three wooden tissues are considered : early wood, late wood and ligneous rays, each one with its own parameters (that is to say 9x3 =27)
First, trough a simple mixture law, the texture $T_{x,}$ giving the thickness of late wood compared to the annual ring thickness as illustrated on figure n°2, allows a valuation of the elastic properties of the homogeneous materiel (in-fi) equivalent to a two layers tissue of early wood (initial) and late wood (final).

$$\frac{1}{E_R^{\inf i}} = \frac{(1-T_x)}{E_R^{\text{initial}}} + \frac{T_x}{E_R^{\text{final}}} \qquad (6)$$

$$E_T^{\inf i} = (1-T_x)\cdot E_T^{\text{initial}} + T_x \cdot E_T^{\text{final}} \qquad (7)$$

$$E_L^{\inf i} = (1-T_x)\cdot E_L^{\text{initial}} + T_x \cdot E_L^{\text{final}} \qquad (8)$$

$E_R^{inf\,i}$, $E_T^{inf\,i}$, $E_L^{inf\,i}$ are the three Young's modulus along three directions R, T and L.

			SSW	**Toward reaction wood**			
				A	**B**	**C**	**D**
Earlywood cell wall	E^m matrix Young modulus	GPa	2	2	2	2	2
	ν^m matrix Poisson ratio		0,3	0,3	0,3	0,3	0,3
	E^f microfibril Young modulus	GPa	62	62	62	62	62
	φ_i microfibril angle MFA in S_2	degree	22	22	22	45	30
	V microfibril volume ratio		0,5	0,5	0,3	0,3	0,3
Early wood tissue	D_{Ti} tangential diameter	µm	30	30	30	30	30
	e_{Ti} tangential cell wall thickness	µm	1,07	1,07	1,07	1,07	1,07
	D_{Ri}/D_{Ti} cell shape parameter		1,25	1,25	1,25	1,25	1,25
	$e_i = e_{Ri}/e_{Ti}$ thickness parameter		0,8	0,8	0,8	0,8	0,8
	$\rho_{initial}$ specific gravity	$g.cm^{-3}$	0,167	0,167	0,167	0,167	0,167
Latewood cell wall	E^m matrix Young modulus	GPa	2	2	2	2	2
	ν^m matrix Poisson ratio		0,3	0,3	0,3	0,3	0,3
	E^f microfibril Young modulus	GPa	62	62	62	62	62
	φ_f microfibril angle MFA in S_2	degree	5,9	5,9	5,9	45	30
	V microfibril volume ratio		0,5	0,5	0,3	0,3	0,3
Latewood tissue	D_{Tf} tangential diameter	µm	35	31	31	31	31
	e_{Tf} tangential cell wall thickness	µm	2,87	4,60	4,60	4,60	4,60
	D_{Rf}/D_{Tf} cell shape parameter		0,43	0,485	0,485	0,485	0,485
	$e_f = e_{Rf}/e_{Tf}$ thickness parameter		1	1	1	1	1
	ρ_{final} specific gravity	$g.cm^{-3}$	0,729	1,1	1,1	1,1	1,1
Ray cell wall	E^m matrix Young modulus	GPa	2	2	2	2	2
	ν^m matrix Poisson ratio		0,3	0,3	0,3	0,3	0,3
	E^f microfibril Young modulus	GPa	60	60	60	60	60
	φ_r microfibril angle MFA in S_2	degree	46	46	46	46	46
	V microfibril volume ratio		0,5	0,5	0,5	0,5	0,5
Ray tissue	D_{Tr} tangential diameter	µm	34,5	34,5	34,5	34,5	34,5
	e_{Tr} tangential cell wall thickness	µm	1,032	1,032	1,032	1,032	1,032
	D_{Rr}/D_{Tr} cell shape parameter		1,18	1,18	1,18	1,18	1,18
	$e_r = e_{Rr}/e_{Tr}$ thickness parameter		1,5	1,5	1,5	1,5	1,5
	P_{final} specific gravity	$g.cm^{-3}$	0,202	0,202	0,202	0,202	0,202
Annual ring	T_x texture		0,512	0,512	0,512	0,512	0,512
	n ray volume ratio	%	2	2	2	2	2
Clear wood Macroscopic properties	Specific gravity	$g.cm^{-3}$	0,45	0,65	0,65	0,65	0,65
	E_R radial Young modulus	GPa	**1**	**1,36**	**1,15**	**3,36**	**2,17**
	E_T tangential Young modulus	GPa	**0,635**	**1,05**	**1,15**	**3,16**	**2,70**
	E_L longitudinal Young modulus	GPa	**13,1**	**18,47**	**11,70**	**9,08**	**11,07**
	E_L/E_R		13,1	13,6	10,19	2,70	5,101
	E_R/E_T		1,57	1,29	1.00	1,06	0,80

Table n°1: Sets of structural and ultra structural parameters of wood tissues used to predict the elastic anisotropy of clear normal Standard Soft Wood (column SSW) and the successive evolutions toward reaction wood (Columns A, B, C and D) (Compression softwood).

Secondly, through another simple mixture law, introducing the parameter n, giving the volume ratio of ray cells, the elastic properties of clear wood are calculated.

$$E_R = (1-n)\cdot E_R^{\inf i} + n\cdot E_R^{rayon} \quad (9)$$

$$\frac{1}{E_T} = \frac{(1-n)}{E_T^{\inf i}} + \frac{n}{E_T^{rayon}} \quad (10)$$

$$E_L = (1-n)\cdot E_L^{\inf i} + n\cdot E_L^{rayon} \quad (11)$$

E_R, E_T, E_L : are the three Young's modulus of clear wood along three directions R, T and L.

2.4 Optimised set of parameters associated to a normal Standard Softwood

Using a set of realistic anatomical parameters as a starting point, chosen through a large literature, and after optimisation of those parameters so that the final values of elastic modulus are as closed as possible to the elastic properties of a standard soft wood [1], the set of structural and ultra structural parameters characterising the Standard Softwood (SSW) are obtained and presented on table 1, column SSW.
For a given specific gravity of the SSW, $\rho = 0,45$ g.cm^{-3}, the target values were:

$E_R = 1,00$ GPa for radial elastic modulus,
$E_T = 0,635$ GPa for the tangential elastic modulus
$E_L = 13,1$ GPa for the longitudinal modulus

The SSW is a clear softwood with a texture $T_x = 0,512$ and a volume faction of rays n = 2%.
The standard early wood has a low specific gravity, $\rho_{initial} = 0,125$ g.cm^{-3}, that is to say a high porosity closed to $P_{0i} = 92\%$, with a microfibril angle in the S_2 sub-layer AMF of $\varphi_i = 22$ degrees.
The standard late wood has a higher specific gravity, $\rho_{final} = 0,729$ g.cm^{-3}, corresponding to a porosity $P_{0f} = 52\%$, with a smaller microfibril angle in the S_2 sub-layer AMF of $\varphi_F = 5,9$ degrees.
This set of parameter, column SSW table 1, will be the starting point of further the discussion.

3. DISTORTION OF SSW PARAMETERS TOWARD THOSE OF COMPRESSION WOOD (CW)

3.1.Structural and ultra structural properties of reaction wood

According to the literature [5], structural and ultra structural properties of reaction wood, here compression wood, differ from those of SSW characteristics.

<u>At the ultra structure level</u>:

compression wood has a lower percentage of cellulose (20 to 30% instead of 50% in normal wood), a greater micro fibril angle AMF inside sub-layer S_2, both in early-wood and late, with a max value of 45 degrees.

<u>At the level of ligneous tissues</u> :

- in early-wood, radial and tangential diameters are not significantly different, $D_{Ri}/D_{Ti} \approx 1$. The cell wall thickness is more or less equivalent to normal early-wood tissue; the cell length is smaller;
- in late-wood, the radial diameter is equal or lightly smaller; the tangential diameter is smaller, so a cell shape parameter D_{Rf}/D_{Tf} higher. The cell wall is significantly thicker, twice both in the radial

or tangential direction, as a consequence the specific gravity of this tissue is twice higher;

- the shape of a cell cross section is more circular, instead of rectangular for normal wood, this induces inter cellular voids ;
- S_3 sub-layer quasi disappears in compression wood ;
- no reported difference between ligneous rays, no significant variation of ray volume ratio.

At the level of annual rings :

The texture is probably higher, with difficulties to identify clearly the transition zone between early and late wood (see figure 3). A higher thickness of annual rings, according to an accelerated production of cells in reaction wood.

At the level of clear compression wood :

Macroscopic properties of compression wood are not very well identified : the specific gravity is 10 or 20% higher, the longitudinal Young modulus E_L is weaker, transverses young modulus E_T and E_R are not clearly identified

3.2.Consequences of properties changes on predicted microscopic elastic properties

Available results are compiled on table 1. Each column A, B, C and D refers to successive changes of parameters and indicate the consequences on elastic characteristics. Those theoretical results are discussed versus parameters of column SSW.

Column A table 1: Increment of specific gravity.
The increment specific gravity from ρ = 0,45 to 0,65 g.cm^{-3} is obtained, column A, through an increment of the cell wall thickness in late wood (e_{Rf} from 2,87 µm to 4,60 µm) and a change of the cell shape parameter (D_{Rf}/D_{Tf} from 0,43 to 0,485).

As expected, an augmentation of the specific gravity induces a significant increment of each clear wood elastic property. The anisotropy is slightly affected by this change.

Column B table 1: Less crystalline cellulose.
A reduction of the percentage of cellulose in reaction wood is illustrated on column B. The change here considered is a decrease from 50% to 30%.

The expected consequence is a lower longitudinal modulus of elasticity E_L , because less cellulose means less reinforcement by microfibrils.

Another effect, more difficult to predict, is an apparent elastic transverse isotropy ($E_R \approx E_T$). This means that the bending behaviour of cell wall, when solicited along tangential direction, has no more apparent influence.

Column C table 1: Higher value of microfibril angle.
Column C corresponds to a change of MFA. Both in early wood and in late wood, the microfibril angle is increased to a maximum value, $\varphi_i = \varphi_f = 45$ °.

As expected, because a larger microfibril angle, the value of the longitudinal Young Modulus E_L falls down from 11,7 to 9,08 GPa, a decrement of 22%.

At the same time, transverse rigidities are significantly enhanced, nearly three times higher. The radial elastic modulus appears greater than the tangential modulus ($E_R > E_T$) as generally observed.

<u>Column D table 1 : Medium increased of the microfibril angle.</u>
Results reported in column D refer to a less important change of the MFA, limited to 30° both in early-wood and late wood.

The decrement of the longitudinal Young modulus E_L is, in this case, significantly smaller. It falls dawn only from 11,7 to 11,07, that is to say 5,4%.

At the same time, the increment of transverse rigidities is limited to two times, and the tangential elastic modulus is greater than the radial Young modulus (E_T = 2,70 GPa > E_R = 2,17 GPa), at the opposite of the relations generally observed experimentally.

4. CONCLUSIONS

The anisotropic elasticity of clear wood is governed by physical and anatomical parameters characterising not only the structure (at the level of the annual ring or of the cell tissues like early-wood or late wood) but also the ultra structure (orientation of microfibrils in the sub-layer S_2 of the cell wall).

Starting from a realistic set of parameters, describing a standard soft wood at different levels, it has been possible to analyse the influences, on the elastic properties of a virtual material, of some successive changes of structural and ultrastructural parameters, allowing the transition from normal wood to compression wood.

Between normal wood and compression wood, the increment of specific gravity, from 0,45 to 0,65 $g.cm^{-3}$, has been concentrated on late wood, mainly through a thickening of the cell wall and an ovalization of the cell cross section.

A deficit of cellulose in compression wood is taken into account by a reduction of the volume ratio of microfibrils (from 50% to 30%).

At last, the effects of an increase of the microfibril angle have been discussed, leading to a fall down of longitudinal Young modulus E_L and a significant increase of transverse elastic properties, with a tendency to isotropy in the transverse plane ($E_R \approx E_T$), depending strongly of the MFA considered.

The effects on E_T and E_R of the microfibrils belonging to S_1 and S_3 are not considered in the model.
We must note that the value of the microfibril's Young modulus, E^f = 62 GPa, suggested by the model is much less than those given in the literature.

The quality and the pertinence of this kind of theoretical results, depend strongly of the relevance of the mechanical modelling; they must be, of course, confronted to experimental evidences. Nevertheless, those predictive mechanical models are efficient tools to imagine new experimental procedures and to interpret experimental results.

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