ISSN: 2977-0041

Review Article

Journal of Material Sciences and Engineering Technology

Multi Scale Modelling of the Hygro-Mechanical Behavior of Rhecktophyllum Camerunense Vegatable Fibers

Noutegomo Boris[1,2*], Betene Ebanda Fabien[2] and Atangana Ateba[2]

[1]*Department of Mechanical and Industrial Engineering, NAHPI School, University of Bamenda Cameroon*

[2]*Laboratory of Mechanic, University of Douala Cameroon*

***Corresponding author**

Noutegomo Boris, Department of Mechanical and Industrial Engineering, NAHPI School, University of Bamenda Cameroon Laboratory of Mechanic, University of Douala Cameroon.

Received: December 09, 2023; **Accepted:** December 20, 2023; **Published:** December 26, 2023

ABSTRACT

The study of rhecktophyllum camerunense (RC) fibers as reinforcement of polymer matrix begin in 2008 and has already demonstrated their ability to replace the glass fibers. In this paper, the influence of humidity on the mechanical behavior of plant fiber is studied and a multiscale model is proposed. The moisture absorption of RC fibers is studied through a multi concentric cylinder model developed based on the work of Marklund. Using mechanical properties of the three main components of natural fibers; cellulose, hemicelluloses and lignines, the mechanical properties and hygroscopic coefficients of layers S1, S2 and S3 of RC fiber are calculated following the relative humidities of 23%, 54% and 75%. The results lead to the conclusion that there is an influence of relative humidity on the mechanical properties whether at the microscopic level of constituents or the mesoscopic scale of layers and the macroscopic scale of RC fiber structure. That influence is negative bacause it drops the mechanical properties of the fiber.

Keywords: RC, Hygroscopic, Swelling Strain, Multiscale Modelling, Mechanical Properties, Hygroexpansion Coefficients

Introduction

In recent years, ecological concern has resulted in an increasing development of natural fibers in industry, to replace glass fibers in composites materials. Their major advantages are mechanics properties comparable to glass fibers, a low density, and a great availability. Moreover, they are renewable and recyclable. But the main inconvenience is their hydrophily due to their weak cristallinity, which contrast to the hydrophoby of matrix used in composite materials. Because of natural ageing, mechanical stresses, temperature and humidity variations of ambient environment, fibers can swell and retract, creating intern stresses and cavities may appear in composites. The effect of absorption of moisture leads to the degradation of fiber- matrix interface region creating poor stress transfer efficiencies resulting in a reduction of mechanical and dimensional properties [1]. To offset this hydrophily, different methods can be developed, for example, by adding a coupling agent which adds a functional group to the cellulose to create hydrophobic film. As the poor resistance towards water absorption is one of the drawbacks of natural fibers, it is more important to study the effects of water absorption on the fiber properties. To understand this phenomenon, many authors use experimental and analytical methods to study the behaviour of mechanical properties of some vegetables fibers exposed to relative humidities of 30, 40, 50, 60, 70% as flax and nettle, flax and sisal, flax [2-4]. Hemp, hemp, sisal, flax, jute, agava to the relative humidities of 10, 25, 50, 80% and flax on the relative humidities of 33% and 60% [4-6]. Many of those works leads to the conclusion that moisture decrease the mechanical properties of natural fibers. The first works on the RC fiber was done by Béakou in 2008 [7]. They used an unstandardized method to extract fibers and the resulting fibers were uniform with almost circular cross-sections. The density of the fiber around 0.947 g/cm3 was found to be very low and chemical analysis revealed that cellulose content was 68.2%. Microscopy observation was used for the measurement of the layer's thicknesses and the microfibril angle of the S2 sub-layer that was 40°. Tensile tests were performed to measure the mechanical properties of the fiber. The Young's modulus 5.8 GPa which was nearly the same as for sisal fiber and elongation at break was very high up to 50%. Many works have also been carried on RC fibers as Chemical and anisotropic characterisation, Moisture sorption isotherms, Study of the diffusion behavior of water on composite, Study of the diffusion behavior of water on fibers and Effect of moisture on the mechanical properties of composite [8-12]. The objective of this study is to analize and understand very well the mechanism of those drawbacks at the level of the chemical constituents (cellulose, hemicellulose and lignine) of the RC fiber and at the different layers S1, S2, S3 according to the relative humidities of 23%, 54% and 75%.

Citation: Noutegomo Boris, Betene Ebanda Fabien, Atangana Ateba. Multi Scale Modelling of the Hygro-Mechanical Behavior of Rhecktophyllum Camerunense Vegatable Fibers. J Mat Sci Eng Technol. 2023. 1(4): 1-6. DOI: doi.org/10.61440/JMSET.2023.v1.17

Material and Methods

Multiscale Modeling

The moisture absorption of RC fibers is studied through a multi concentric cylinder model developed based on the work of Marklund [13,14]. Using mechanical properties of the three main components of natural fibers; cellulose, hemicelluloses and lignines, the mechanical and hygroscopic coefficients of layers S1, S2 and S3 of RC fibers are calculated. They depend on the volume fraction of these three components and on the relative humidity of hemicelluloses and lignines. In this study, cellulose is considered to be 100% crystalline. Finally, a finite element model based on the result of experiments and an analytical model is developed in order to determine the mechanical behavior of a RC fiber following the relative humidities of 23%, 54% and 75%.

Microfibril UC Hygroelastic Layer Properties Softwood Fiber

The fiber wall layer averaged properties will be modeled starting from cellulose, hemicellulose and lignin chemical constituent. The RC fiber properties will then be calculated from the proprties of The fiber wall layer S1, S2 and S3 as mention on figure 1. As many micromechanical parameters on RC fibers are not yet obtained and the decision was made to use some elastic properties of wood as shown in Table 1.

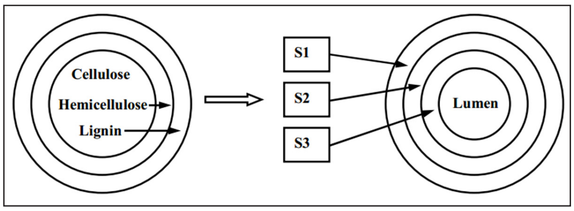

Figure 1: Multiscale modeling of a softwood fiber using the concentric cylinder model

Table 1: Assumed engineering constants of the wood polymers (dry conditions)

Phase	Material behavior	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	v_{12}	v_{23}
Cellulose	Transversely isitropic	150	17.5	4.5	0.1	0.5
Hemicellulose	Transversely isitropic	8	3.4	1.2	0.33	0.43
lignin	isitropic	6			0.33	

The RC fiber will be modeled as an assembly of long coaxial cylinders with high aspect ratio. This means that the stress transfer zone extends only over a small part of the interface and perturbation effects at fiber ends may be neglected.

The Concentric Cylinder Model

Micromechanical models for long fiber composites have been developed by Hashin and Rosen, Hashin and Christensen and Lo considering the constituents as concentric circular cylinders [15-17]. In the stiffness expressions for an isotropic hollow circular fiber composite were developed. The basic idea was that the entire cross-section of a composite material consists of many concentric pair cylinders with different outer diameters, but all having the same fiber volume fraction [15]. The limitation with Hashin's micromechanical model is that it renders only upper and lower bound for the transverse shear modulus. The limitation is related to the used homogenized boundary conditions in displacements or in tractions which do not exactly correspond to the conditions on the cylindrical boundary in a homogenized material. This problem was solved by Christensen and Lo using a generalized self-consistent scheme [17]. They considered an infinite effective composite with unknown shear modulus and a cylindrical sub-domain in it replaced by an equivalent fiber matrix microstructure. Albeit proven very useful in many practical applications, these models may not be suitable for modeling natural fiber composites since they are limited to isotropic and transversely isotropic phase materials whereas natural fibers are at least orthotropic in cylindrical axes with different properties in the radial and in the hoop direction. Therefore, an analytical micromechanical model valid for orthotropic phase materials and for an arbitrary number of phases was developed to study the effect of various constituent stiffness properties on an aligned wood fiber composite[18].

Determination of Hygroexpansion Coefficients

The free hygroexpansion of wood fibers is a well known phenomenon. Moisture absorption leads to an increase in moisture weight content and dimensional changes of the fiber as a consequence. In the linear elasticity of orthotropic materials these changes are assumed to be proportional to the moisture content change and three different constant coefficients of proportionality called hygroexpansion coefficients (β_j) characterize the relative dimensional changes in three directions of the material symmetry. As the result of phase swelling only normal stresses and strains develop, all shear components being zero, and the elastic stress-strain relationship may be written:

$$\sigma = C_{ij}(\varepsilon_j - \beta \Delta M) \quad (1)$$

Cij is the stiffness matrix with usual notation and ΔM is the moisture weight content change. For an axi-symmetric problem in a particular case of loading when all shear stress components are equal to zero, the only non-trivial equilibrium equation is

$$\frac{\partial \sigma_\gamma}{\partial \gamma} + \frac{\sigma_\gamma - \sigma_0}{\gamma} = 0 \quad (2)$$

By using Eq. (1), Eq. (2) and the strain to radial displacement relationship the displacement field equation for one cylinder may be set up and solved with following result:

$$u_r = A_1 r^{\alpha} + A_2 r^{-\alpha} + \frac{C_{13} - C_{12}}{(1-\alpha^2)C_2}\left(\varepsilon_1 r - \frac{H\Delta M}{C_{13} - C_{12}} r\right) \quad (3)$$

where

$$\alpha^2 = \frac{C_{33}}{C_{22}}, \quad H = (C_{13} - C_{12})\beta_1 + (C_{23} - C_{22})\beta_r + (C_{33} - C_{23})\beta_\theta \quad (4)$$

A_1 and A_2 are unknown constants and ε_1 is the constant strain in axial direction as a result of phase swelling. For a composite cylinder Eq. (3) is generalized to N-phases with the requirement that the displacement and stress expressions have to satisfy continuity conditions on all interfaces, i.e. the solutions obtained for each phase separately must satisfy the following conditions: (i) Radial displacement must be zero on the symmetry axis; (ii) Displacement and radial stress continuity conditions at all interfaces; (iii) Zero radial stress at the outer boundary $\gamma = \gamma_N$

of the cylinder assembly. In case of free swelling the constant strain in axial direction must result in zero average stress in that direction. It is then realized that the unknown constants A_1^K and A_2^K for k 1,..., N can be determined by setting up and solving a system of linear algebraic equations. The problem is conveniently solved by using ε_1 as a numerical parameter for the requirement of zero axial stress. For every value of ε_1 the system of linear equations is solved and checked whether zero average stress in axial direction (with required accuracy) is obtained. When ε_1 have been determined the hygroexpansion coefficients in longitudinal direction β_L and transverse direction β_T of the cylinder assembly may be calculated from

$$\beta_L = \frac{\varepsilon_1}{\Delta m_{avg}} \quad \beta_T = \frac{\varepsilon_T^{avg}}{\Delta M_{avg}} = \frac{u_r(r_N)}{r_N \Delta M_{avg}} \tag{5}$$

The average moisture content of the analyzed assembly ΔMavg is determined using the rule of mixtures. For further detail regarding derivations and explicit expression for solving the hygroexpansion coefficients the reader is advised to [18].

Helical Fiber Structure

In reality a RC fiber cell wall layer is at least an orthotropic material in its local system of coordinates. However, if the concentric cylinder assembly model is used to calculate its properties using the multiscale approach starting from the properties of fiber cellulose, hemicellulose and lignin the cell wall layer will be transversely isotropic in the local coordinate system. The theory presented in this section is valid for more general materials with orthotropic layer properties in their corresponding local coordinate systems. Notation and orientation of local and global axes is shown in Figure. 2.

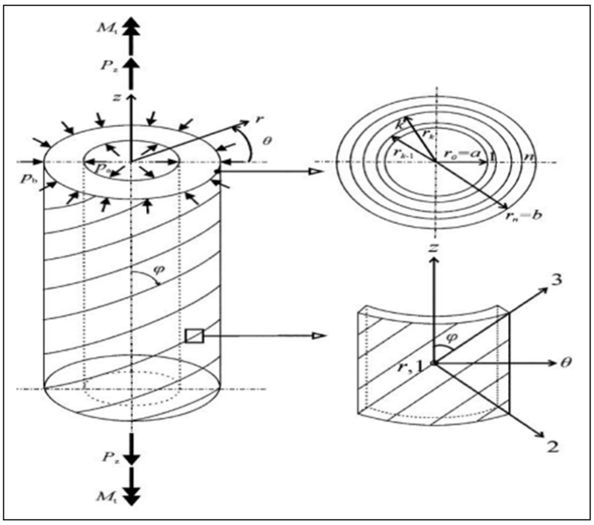

Figure 2: Schematic drawing of a cylindrical cell wall layer in a) global view, b) detail of the layer showing the relationship between local (L, T, r) and global coordinates (z, φ, r).

In the global system of coordinates the layer has only one symmetry plane, which is the (z,φ)-plane, and the material has a monoclinic symmetry in these coordinates. Expressions for radial displacement and the relevant stresses and strains are given in detail in [18]. The radial displacement for the k-th sub-cylinder is

$$u_0^k = A_1^k r^{\alpha_k} + A_2^k r^{-\alpha_k} + \varepsilon_1 \alpha_1^k r + D_1 \alpha_2^k r^2 \tag{6}$$

A_1^K and A_2^K are unknown constants, α_K, α_1^K and α_2^K are known functions of the k-th phase elastic constants. ε_1 is the strain in z-direction and is coordinate independent (constant). D_1 is related to the rotation of the cylinder assembly due to monoclinic material properties. As in the previous discussion regarding determination of the hygroexpansion coefficients displacement and stress continuity conditions have to be satisfied at the interface between two sub-cylinders (layers) with indexes k and k + 1. In addition the center phase must be either isotropic or transversely isotropic. It can be shown that using the appropriate displacement and stress continuity conditions will lead to the following relationships between constants to be determined:

$$A_1^k r_k^{\alpha_k} + A_2^k r_k^{-\alpha_k} - A_1^{k+1} r_k^{\alpha_{k+1}} - A_2^{k+1} r_k^{-\alpha_{k+1}}$$
$$= \epsilon_1 r_k \left(\alpha_1^{k+1} - \alpha_1^k\right) + D_1 r_k^2 r_k \left(\alpha_2^{k+1} - \alpha_2^k\right) \tag{7}$$

$$A_1^{k+1} \beta_1^{k+1} r_k^{\alpha_{k+1}-1} - A_2^{k+1} \beta_2^{k+1} r_k^{-\alpha_{k+1}-1} = \epsilon_1 \left(\beta_3^{k+1} - \beta_3^k\right) + D_1 r_k \left(\beta_4^{k+1} - \beta_4^k\right) \tag{8}$$

β_1 - β_4 are known functions of the k-th phase elastic constants [18]. The external boundary of the N-cylinder assembly is free of radial tractions:

$$\sigma_r(r_N) = A_1^N \beta_1^N r_N^{\alpha_N - 1} + A_2^N \beta_2^N r_N^{-\alpha_N - 1} + \epsilon_1 \beta_3^N + D_1 \beta_4^N r_n = 0 \tag{9}$$

The unknown constants A_1^K and A_2^K for k=1,..., N can be determined by setting up and solving a system of linear algebraic equations using Eq. (7-9). If no rotation of the cylinder assembly is allowed then = 0 and the system of linear algebraic equations is readily solved using a constant . If the assembly is allowed to rotate freely then is unknown and must be determined from the requirement of zero average torque according to

$$T_{z\varphi}^{av} = 2\pi \sum_{k=1}^{N} \int_{r_{k-1}}^{r_k} r^2 \sigma_{z\varphi}^k dr = 0 \tag{10}$$

Insertion of the expression for $\alpha_{z\varphi}^K$ in Eq. (10) give the condition needed to determine D_1. The problem is conveniently solved by using D_1 as a numerical parameter. For every value of D_1 the system of linear equations is solved and Eq. (10) used to check whether zero average torque (with required accuracy) is obtained. Poisson's ratio may be calculated from the displacement of the outer cylinder boundary, and the associated z-axis force can be used to define the apparent elastic modulus of the assembly:

$$E_z = \frac{\sigma_z^{av}}{\epsilon_1} = \frac{2}{\epsilon_1 r_N^2} \sum_{k=1}^{N} \int_{r_{k-1}}^{r_k} r \sigma_z^k dr \qquad \nu_{2r} = -\frac{u_0(r_N)}{r_N \epsilon_1} \tag{11}$$

Results and Discussion

Hygroelastic Properties

Firstly the microfibril UC hygroelastic properties were calculated. The assumed volume fractions of the RC fiber were: S2 and S3 layers 49% volume fraction of cellulose, 27% hemicellulose and 24% lignin. The S1 layer had 20% volume fraction of cellulose, 15% hemicellulose and 65% lignin. These values are for dry material, but since hemicellulose and lignin will absorb moisture and swell for some given relative humidity (RH) their volume fractions will change. The stiffness of hemicellulose and lignin will also change. By using the data on moisture absorption and the stiffness moisture dependence presented by Cousins [19]. The hygroelastic properties and the new volume fractions for the microfibril UC were determined. The hygroexpansion coefficients β_l and β_T were determined based on the assumptions made by Cave that β_{CE}= 0 in all directions and β_{HC}= 0.5 in transverse directions and β_{LI}= 0.33 in all directions [20]. Thus cellulose is believed to stay unaffected by moisture and the swelling in longitudinal direction for hemicellulose is considered to be insignificant. These are rather crude assumptions. However, due to lack of other data at hand these values will suffice for modeling purposes at time being.. Table 2 shows the obtained result for 23%, 54% and 75% RH calculated using the CC-model. We note generally that the mechanical properties of the layers S1, S2, S3 for a relative humidity of 23% are greater than 54% and even more for 75%. Figures 3, 4, 5, 6 present the variations of these properties.

Table 2: Hygro-mechanical properties of layers for different relative humidities obtained by CC-model

	Relative humidity (%)					
	23		54		75	
Properties	S1	S2-S3	S1	S2-S3	S1	S2-S3
EL (Gpa)	29.98	74.42	28.17	72.49	26.22	71.03
ET=ER (Gpa)	6.53	8.11	4.92	6.30	3.08	4.26
GLT=GLR (Gpa)	2.36	2.57	1.63	2.38	1.17	1.24
GTR (Gpa)	3.002	2.68	1.66	2.26	1.18	1.32
νLT= νLR	0.295	0.219	0.280	0.211	0.288	0.201
νTR	0.412	0.544	0.445	0.460	0.450	0.44
βL	0.026	0.011	0.024	0.008	0.005	0.007
βT= βR	0.580	0.507	0.549	0.488	0.530	0.468

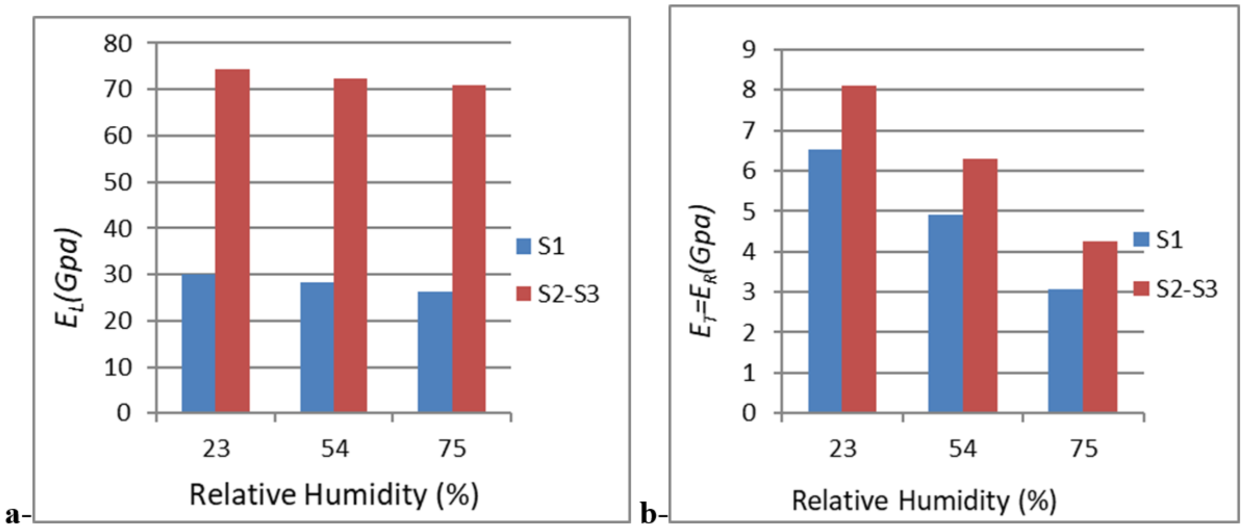

Figure 3: Evolution of the modulus of elasticity as function of relative humidity: a-longitudinal and b-tangential or radial.

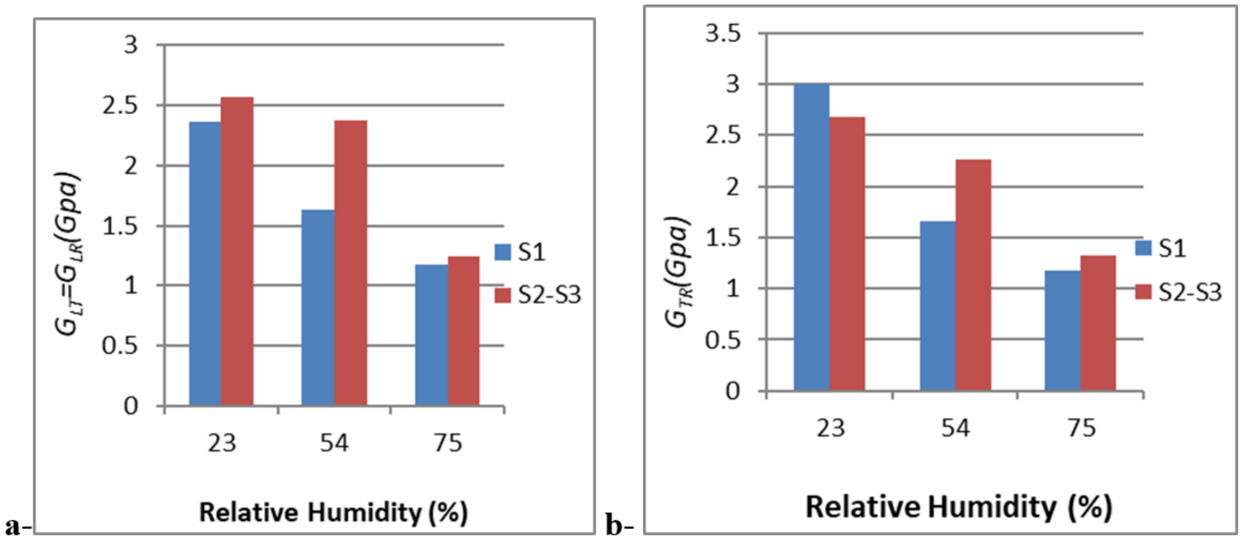

Figure 4: Evolution of the shear modulus as a function of relative humidity: a-G_{LT}=G_{LR} and b- G_{TR}

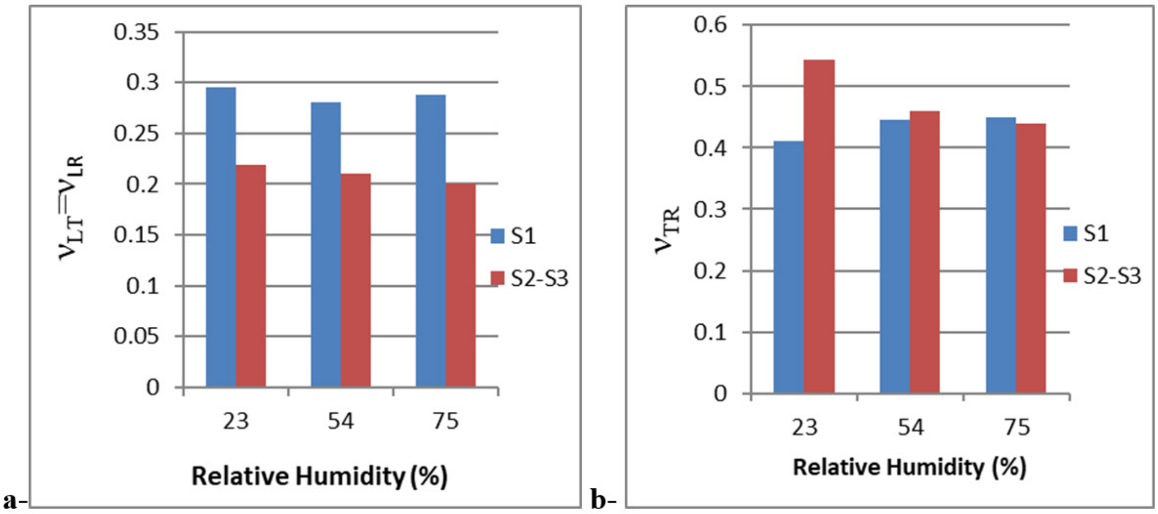

Figure 5: Evolution of the poison ratio as function of relative humidity: a- $\nu_{LT}=\nu_{LR}$ and b- ν_{TR}

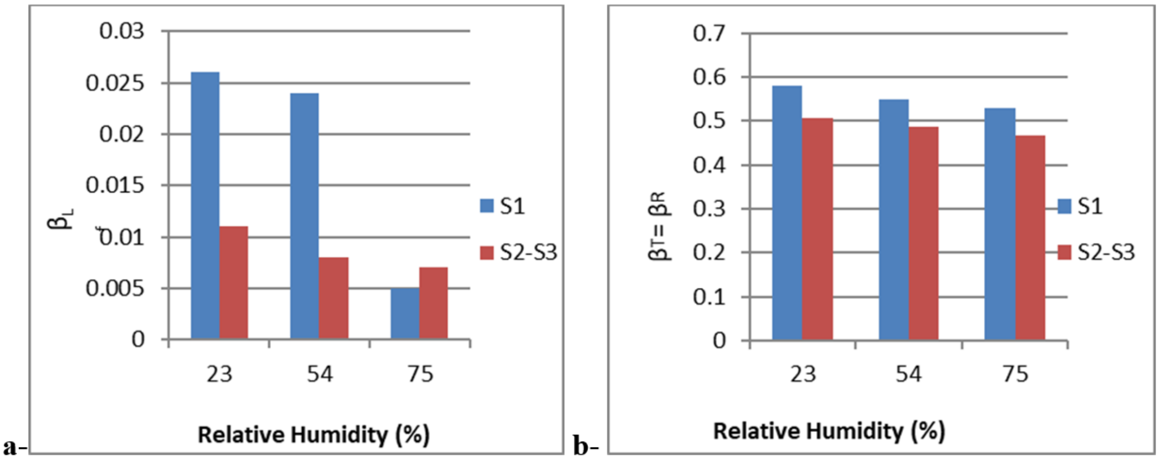

Figure 6: Evolution of the hygroexpension coefficient as a function of relative humidity: a-longitudinal and b-tangential or radial.

The longitudinal modulus of elasticity of the S1 layer drops by about 7.43% when going from 23% to 54% relative humidity then 6.42% when going to 75%. That of layers S2-S3 is very little affected with a drop of 2.66% then 2.05% for the same ranges relative humidities. This would be due to the high rate of cellulose available in these two sub layers. The radial modulus of layer S1 drops by 32.72% then by 59.74%. For the layers S2-S3 there is a drop of 28.73% then 47.88%. This shows that the influence of moisture on the mechanical properties at the level of the sub-layers resulting in a decrease in these properties with increasing relative humidity. This drop is also observed at the level of the shear moduli when the relative humidity increases. For the layer S1 it is 44.78% then 39.31%. For layers S2-S3 the drop goes from 18.58% then to 71.55%. Those first results lead to the conclusion that there is an influence of moisture on the mechanical properties whether at the mesoscopic scale of layers or macroscopic scale of RC fiber structure. Those results are in conformity with those encountered in the literature for exemple the sisal, jute, hemp, flax and nettle [2-6]. That bring us to the conclusion that the RC fibers like many of fibers should be treated before using them in composite materials. This treatment will decrease the hydrophilic behavior of fiber, encrease his dimensional stability insite the composite and fiber-matrix adhesion properties. We obseved that moisture don't affect the poison ration coefficient nomatter. Therefore the hygroexpension have been wery well affected. We noted a great decreasing concerning the longitudinal direction and more in layer S1. This should be explain by the fact that the S1 layer has small thickness and then poor content of cellulose. The decrease in transverse and radial direction are not very pronounced.

Conclusion

The objective of this paper was to present micromechanical models that are suitable for parametric studies of fiber properties. Multiscale modeling of hygroelastic properties has been performed for RC fiber using concentric cylinder model developed based on the work of Marklund. The cell wall was modeled regarding each individual layer as a concentric cylinder. Mechanical properties of the three main components of natural fibers; cellulose, hemicellulose and lignine, the mechanical and hygroscopic coefficients of layers S1, S2 and S3 of RC fibers are calculated. We note generally that the mechanical properties of RC fibers drop with the moisture as many of them encounter in the litterature. That bring us to the conclusion that RC fibers should be treated before using them in composite materials to conserve his mechanical properties.

Declarations

Ethics Approval and Consent to Participate: Not applicable

Consent for Publication: Not applicable

Availability of Data and Material: All data generated and/or analysed during this study are included in this research article

Competing Interests: The authors declare that they have no competing interests.

Funding: Individual

References

1. Dhakal H, Zhang Z, Richardson M. Effect of water absorption on the mechanical properties of hemp fiber reinforced unsaturated polyester composites. Composites Science and Technology. 2007. 67: 7-8.
2. Davies GC, Bruce DM. Effect of Environmental Relative Humidity and Damage on the Tensile Properties of Flax and Nettle Fibers. Textile Research journal. 1998. 68: 623-629.
3. Cruz VCA, Nóbrega MMS, Silva WP, Carvalho LH, Lima AGB. An experimental study of water absorption in polyester composites reinforced with macambira natural fiber. Mat.-wiss. u. Werkstofftech. 2011. 42S: 979-984.
4. Stamboulis A, Bailli CA, Peijs T. Effects of environmental conditions on mechanical and physical properties of flax fibers. Composites: Part A. 2001. 32: 1105-1115.
5. Symington MC, Banks WM, David WO, Pethrick RA. Tensile Testing of Cellulose Based Natural Fibers for Structural Composite Applications. Journal of composite materials. 2009. 43: 1083-1108.
6. Roudier A. Analyse multi-échelles du comportement hygro-mécanique des fibres de lin. Autre. Université Blaise Pascal - Clermont-Ferrand II, Français. 2012.
7. Béakou A, Ntenga R, Lepetit J, Atéba JA, Ayina LO. Physico-chemical and microstructural characterization of "rhectophyllum camerunense" plant fiber. Composites Part A: Applied Science and Manufacturing. 2008. 39: 6774.
8. Ntenga R. Modélisation multi-échelle et caractérisation de l'anisotropie élastique des fibres végétales pour le renforcement de matériaux composites. Vegetal Biology. Université Blaise Pascal - Clermont-Ferrand II, Université de Yaoundé. 2007.
9. Noutegomo B, Betene EF, Atangana A. Modelling moisture sorption isotherms of Rhecktophyllum camerunense vegetable fiber, European Journal of Pure and Applied Chemistry. 2017. 4: 33.
10. Betene E, Noutegomo B, Atangana A. Study of the diffusion behavior of water vapor sorption in natural fiber: Rhecktophyllum camerunense. Indian Journal of Engineering. 2018. 15: 143-150.
11. Noutegomo B, Betene EF, Atangana A. Study of the diffusion behavior of water vapor sorption in natural fber composite: Plaster/Rhecktophyllum camerunense A. MOJ App Bio Biomech. 2019. 3: 12-16.
12. Noutegomo B, Betene EF, Atangana A. Effect of moisture on the mechanical properties of Rhecktophyllum Camerunense Natural Fiber/ Plaster Composites. Journal of Material Sciences & Manufacturing Research. 2020. 1: 1-7.
13. Marklund E, Varna J, Neagu C, Gamstedt EK. Stiffness of aligned woof fiber composites: Effect of microstructure and phase properties, Composites Materials, 42, n°. 2008. 22: 2377-2405.
14. Marklund E, Varna J. Modeling the hygroexpansion of aligned wood fiber
15. Hashin Z, Rosen BW. The elastic moduli of fiber-reinforced materials. Journal of Applied Mechanics. 1964. 31: 223-232.
16. Hashin Z. Analysis of Composite Materials - a survey. Journal of Applied Mechanics. 198. 50: 481-505.
17. Christensen RM, Lo KH. Solutions for effective shear properties in three phase sphere and cylinder models. Journal of the Mechanics and Physics of Solids. 1979. 27: 315-330.
18. Marklund E. Modeling the mechanical performance of natural fiber composites. Doctoral thesis. Department of Applied Physics and Mechanical Engineering, Division of Polymer Engineering, Luleå University of Technology, Luleå, Sweden, 2007. composites, Composites Science and Technology, 2009. 69: 1108-1114.
19. Cousins WJ. Young's modulus of hemicellulose as related to moisture content, Wood Science and Technology. 1978. 12: 161-167.
20. Cave ID. Modelling moisture-related mechanical properties of wood Part I: Properties of the wood constituents. Wood Science and Technology. 1978. 12: 75-86.