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Numerical modelling of hygro-mechanical behavior of Rhecktophyllum Camerunense vegatable fibers

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Abstract. Indeed the influence of humidity on the mechanical behavior of *Rhecktophyllum Camerunense* (RC) vegatable fiber was studied using numerical modelling and simulation. This method was used to investigate the hygromechanical caracteristics of the vegetable fiber that should be difficult to obtain experimentally. Another goal is to compare the results obtained experimentally and analytically in others works. The Finite Element Analysis using ANSYS sofware enables us to discretize a continuous problem and obtain an approximated solution. The Modeling Geometry adopted was an assembly of three concentric cylinders representing the sublayers S1, S2 and S3 of the fiber. The numerical model developed is a decoupled hygromechanical model. Thus the first stage of this model concerns the consideration of hygroscopy by simulating the diffusion of water within the material. Secondly, the mechanical calculation is carried out by taking as loading the results of the purely hygroscopic calculation, expressed in the form of hygroscopic fields. Identification of input parameters for the numerical simulation was found in literature. The results coroborated with the ones of literature and shown that humidity decrease the mechanical properties of RC vegetable fiber.

Keywords: RC fibers / hygroscopic / swelling strain / FEM / mechanical properties / ANSYS

1 Introduction

The demand for bio-based materials in semi-structural and structural application is constantly growing to conform to new environmental policies enacted in Europe and worldwide which try to replace conventional oil-based polymers and composites. Natural fibers reinforced composites meet an important success because of their interesting specific mechanical properties, availability and reasonable price compared to conventional glass fiber reinforced composites [1]. The interest in natural fibre reinforced polymer composites is growing rapidly due to its high mechanical performances, low cost and ease of processing. Natural fibers are relatively cheap, pose no health hazards and offer solution to environmental pollution by finding new uses for waste materials. However, the hydrophilic nature of these vegatable fibers results in a poor durability when exposed to humidity and temperature [2]. Their applications are still limited due to several factors like moisture absorption, poor wettability and large scattering in mechanical properties [3,4]. Natural fibers and its composites are hydrophilic materials. Moisture content in fiber composites significantly affects their physical and mechanical properties. The absorbed moisture results in to the deterioration of mechanical properties since the water not only affects the unfilled polymer matrices physically and/or chemically but also attacks the hydrophilic natural fiber as well as the fiber-matrix interface. To understand this phenomenon, many authors used experimental investigations to study the behavior of mechanical properties of some vegetables fibers exposed to relative humidities of 30%, 40%, 50%, 60%, 70% as flax and nettle [5], flax and sisal [6], flax and Hemp [7], hemp, sisal, flax, jute, agava to the relative humidities of 10%, 25%, 50%, 80% [8] and flax on the relative humidities of 33% and 60% [9]. Many of those works leads to the conclusion that moisture decreases the mechanical properties of natural fibers. Few of them mentionned that the moisture doesn't affect the mechanical properties of natural fibers. The experimental investigations are very important because they are closed to the reality. Experiments also have some limits because of the high cost. They require specialized ultramodern laboratories with well-trained staff. They also consume a lot of time and energy. The other limitation lies in the fact that majority of the hygro-mechanical

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characteristics are only known at the macroscopic scale of the fiber and its microstructure at the scale of chemical constituents and sub-layers are difficult to obtain. To complete these shortcomings resulting from the experimental method, the use multiscale modeling method whether analytical or numerical os very important. Despite the fact that this method is based on idealized fibres, a better agreement has always been observed in comparison with the experimental results. Modelling method is highly dependent on experiments because the datas needed for simulation comes from experimental results. Besides, the evolution of their mechanical properties in service conditions can be predicted with numerical simulations that rely on experimental results [10,11]. Having a numerical model offer the opportunity to assess the influence of many parameters during aging. Plant fibres exhibit a hierarchical structure, leading to complex mechanical. Deciphering the origins of this behaviour in terms of physical phenomena requires exploring different scales from millimetres to the molecular scale. Consequently, numerical approaches such as the finite element analysis (FEA) are gaining increasing interest as complements to tedious experimental characterization. The great variability of plant fibres and the need to take into account a complex hierarchical structure led to the use of numerical methods such as the finite element analysis. The FEA enables us to discretize a continuous problem and obtain an approximated solution. Analytical and numerical work on plant fibres originated from wood in the 1950s and was extended to plant fibres such as flax and hemp in more recent years. Industrial interests have most likely been conducting the research in the area of wood, and emerging numerical works on plant fibres is still constrained by the difficulty of obtaining experimental datas to corroborate the models. Researchs on hygromechanical behavior of composite based on vegetables are abondants while the modelling of plant fibres remain an open challenge. The littérature on the domain is very poor. The first step is to define the physical system to be analysed and convert in a mathematical model that can be either mesh-based (FEA) or meshless (molecular dynamics). The discretisation of the mathematical model leads to a finite element model. Within the context of fibre mechanical modelling, the procedure is the following: defining the fibre geometry, meshing the geometry with structural elements, defining the boundary and loading conditions (displacement-based and force-based), specifying the material model (isotropic, anisotropic, elastic, elasto-plastic, etc.), and performing the analysis (static, dynamic, transient). Under the assumption of linear elasticity, the calculations are based on the generalized Hooke's law predicting deformations caused by an arbitrary combination of stresses in a material. The young modulus is the initial slope of the curve stress in fonction of strain as presented in equation (1).

$$\mathrm{E} = \tan\alpha = \frac{\Delta\sigma}{\Delta\varepsilon}\,\mathrm{in\,GPa} \tag{1}$$

Δσ: variation of stress in MPa; **Δε**: variation of strain in %.

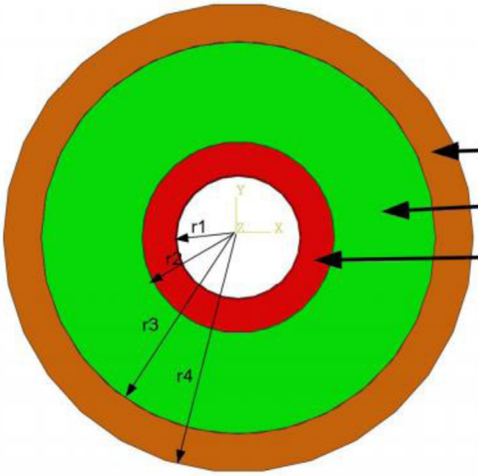


Fig. 1. Modeling of an RC fiber, S1 is in brown, S2 in green and S3 in red (cylindrical geometry).

The number of independent variables is reduced depending on the symmetry of the system. More complex behaviour laws, taking into account viscoelasticity or plasticity, for instance, can be implemented depending on the material. After solving the equation system using either direct or indirect solvers, the convergence and correctness of the model are checked, and these steps might require refinement. The final output is an approximate solution of the initial problem. Experimental data are required at different steps to strengthen the model: at the nanoscopic or microscopic scale to help define a realistic model and at the macroscopic scale to check the correctness of the model. Moreover, fibre geometries have to be implemented in the model. Neagu et al. [12] developed a multilayer finite element model to investigate the link between the MFA and hygroelastic behaviour of wood fibres. They studied different boundary conditions and found that constrained fibres exhibit a stiffer response, resembling the behaviour of plant fibres constrained by their neighbours. Changes in the MFA were correlated with changes in the compliance values. The dominating deformation mechanism under moisture content changes was the twisting of the fibres. The model was further developed by Joffre et al. [13] using a 3D reconstruction of the S2 layer obtained by X-ray microtomography. The hygroexpansion coefficients were estimated by comparing the predicted and experimental geometries in the wet state. They minimized the geometrical approximation, but only the elastic behaviour was studied. Finally, a multi-scale finite element analysis was developed by Saavedra Flores et al. [14], covering the tensile behaviour from microfibrils to bulk Palmetto wood. The evaluation of moisture content is based on the equation (2). Specimen are dried in an oven and expose to humidity. The mass is mesured at progressive intervals of time untill saturation. Therefore the kinetic absorbtion of the specimen can be realized by a curve of moisture content in function of time.

$$\mathrm{M} = \frac{m_o - m_i}{m_o} \tag{2}$$

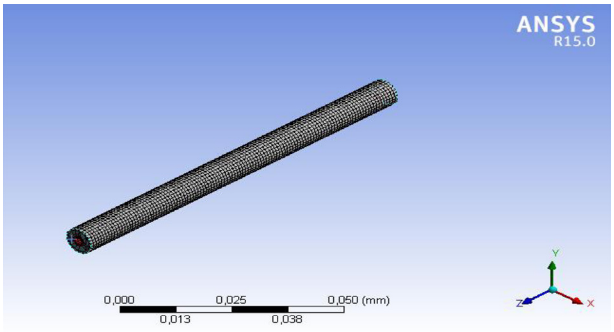


Fig. 2. Mesh structure of the elementary fiber.

m_o is the mass of the dry specimen; m_i is the mass of the wet specimen.

Research are still going on new fibers in order to understand their caracteristics such as the hygromechanical behaviour. Amoungt them we have *Rhecktophyllum Camerunence* fibers on which the researchs started in 2008. The physical, chemical and microstructural characterization were carry out [15]. The modelling of the moisture sorption isotherm of the Rhecktophyllum Camerunence (RC) fiber at 23 °C by using the BET, GAB and DLP models where also studied [16] and his diffusive behavior was investigated to determine the diffusion coefficient [17]. The experimental hygromechanical study of this fiber were also carry out [18]. The mathematical modeling of hygromechanical were also studied at the level of chemical constituant of the fiber to undetstand the behavior of the sub-layers [19]. This modeling was based on the works of Marklund [20,21]. The aim of this study is to undesrtand the hygro-mechanical behavior of RC fibers using the FEA sofware ANSYS in order to validate the results obtained experimentally.

2 Methodology

2.1 Modeling geometry adopted

This paragraph presents in detail the numerical model designed under the finite element simulation software ANSYS. The numerical model developed is a decoupled hygromechanical model. Thus the first stage of this model concerns the consideration of hygroscopy by simulating the diffusion of water within the material. For this, we used the diffusion properties and the boundary conditions imposed inside and outside the fiber and which correspond to the water content at saturation of the material. Secondly, the mechanical calculation is carried out by taking as loading the results of the purely hygroscopic calculation, expressed in the form of hygroscopic fields. They are obtained at saturation of an elementary fiber.

For the fiber we consider an ideal geometry (Fig. 1) corresponding to an assembly of concentric cylinders representing the sub-layers S1, S2 and S3 taking into account the fact that the RC fiber has a large circularity. The average diameter of the fiber is 20 μm, it comes from the literature [15]. The lumen represents 20% of the radius, the sub-layers S1, S2 and S3 represent respectively 10%, 85% and 5% of the total fiber thickness. The circles, thus modeled are extruded over a length of 0.1 mm.

Between each sub-layer we have three interfaces represented by the radius $r_{2,}$ and r_4. For interior and exterior are represented by the radius r_1, and r_5 which are respectivelly the radius of lumen and fiber. For boundary conditions we have continuities of displacements and stresses in the interfaces S3 – S2 and S2 – S1 to avoid slips on x, y, z directions.

2.2 Mesh and hygroscopic loading

As soon as plant fibers are brought into contact with the ambient air, an absorption or desorption phenomenon which depends on the water content within the fibers and on the ambient humidity occurs at the level of the fibres. But this phenomenon is not instantaneous. This is why the hygroscopic loading is carried out by a transient model. The element type chosen is the Solid70 element, which is an 8-node 3D element and has temperature as its degree of freedom. We assume that there is a slight variation in temperature between the inner and outer walls. In our case, the temperature corresponds to the humidity for the fiber. The finished geometry is then meshed by choosing all the areas (Fig. 2). The elements have a length of 0.1 mm in the longitudinal direction. The corresponding sub-layer is then associated with each volume. When the mesh has been carried out as presented on Figure 2, the hygroscopic loading is applied to the nodes of the mesh belonging to the interior and exterior edges of the geometry studied.

2.3 Obtaining macroscopic flexibility constants

The purpose of the numerical model is to determine the macroscopic flexibility tensor of the RC fiber from the hygro-mechanical properties of the sub-layers. For this, it is necessary to apply different boundary conditions to the fiber according to the constants to obtain. Then the homogenization is done according to a mechanical calculation whose loading is the hygroscopic field determined in the preceding paragraph. At the beginning of the mechanical calculation, it is necessary to pass from the hygroscopic part of Ansys to the structure part thus changing the Solid70 element to Solid185, which is a 3D structural element with 8 nodes or a layered element.

2.4 Identification of input parameters for the numerical simulation

Mechanical properties of the sub-layers S1, S2 and S3 that will be used in our model to have the properties at the macroscopic level of the fiber should ccme from the literature rewiew. Some of them have been determined experimentally and others by modelling and simulation. One of the parameter is the ticknesses of sub-layers as mention in Table 1. The thicknesses mentioned in this table are those obtained from TEM observations of the RC fiber. The density is also needed and the value is 0.9g/cm^3 determined experimentally [15].

Table 1. Thicknesses of sub-layers [16].

Sub-layers	S_1	S_2	S_3
Thicknesses (μm)	0.53	1.6	0.6

Table 2. Mechanical properties of the sub-layers plant fiber constituents in the dry state [21].

Constituents	Mechanical behavior	E_L (GPa)	E_T (GPa)	G_{LT} (GPa)	ν_{LT}	ν_{TR}
Cellulose	Isotrope transverse	150	17.5	4.5	0.1	0.5
Hemicellulose	Isotrope transverse	8	3.4	1.2	0.33	0.43
Lignin	Isotropic	6			0.33	0.33

The mechanical properties of fibers were determined in the dry state. They are presented in Table 2.

For simulation it is necessary to know the diffusion coefficient of water in the RC fibers and the datas are presented in Table 3. They have been obtained experimentally using Fick's law [17].

Another parameter is the microfibril angle (MFA) of each layer regrouped in Table 4.

The only data in the literature concerning the microfibrils angle of the RC fiber is the value of the S2 sub-layer [15]. The value of angle in the S1 and S3 sublayers are taken from the wood fiber data [20]. We also need to know the water content to apply to the inner and outer edges of the geometry. This water content was determined experimentally following hygroscopic tests carried out on the RC fiber [16]. The second part of the numerical model is based on the mechanics and therefore on the properties of each sub-layer in its orthotropy reference frame. These properties were determined in literature [15].

3 Results and discussion

3.1 Hygroscopic properties at the macroscopic scale for different relative humidities

The applied humidity corresponds to the water content at saturation for a given relative humidity. Figure 3 gives the adsorption kinetics for an elementary fiber modeled at a relative humidity of 75%, which corresponds to a water content at saturation of 10.84%. This water content is close to the 10% that was determined experimentally [16]. The saturation time is instantaneous. It is 0.15s instead of 7h determined experimentally. Experimentally the fibers are dried in an oven and exposed to humidity. The moisture taken are mesure with a balance at intervals of time untill the mass does not vary again. We observed that no matter the relative humidities, they increase from zero which is the dry state untill the saturated point and from there the curve is flat because the mass does'nt vary again. The same evolution is observed in the modelling curve and it just take few secondes. only the curve of 75% relative humidity is presented.

Table 3. Diffusion coefficients of RC fiber as function of relative humidity [18].

Humidité relative (%)	Coefficient de diffusion D (mm^2/s)
23	0.68E-10
54	0.86E-10
75	1.14E- 10

Table 4. Microfibril angle of sub layers according to longitudinal axis [16,21].

Sub-layer	S_1	S_2	S_3
Microfibril angle	−80	+40	+60

The hygroscopic distribution represented by Figure 4 for the relative humidities of 23, 54, 75% is not uniform throughout the fiber, but all the values are close to the water contents determined experimentally and therefore the fiber will be considered as saturated in water. Table 5 presents the water content values obtained by our modelling.

3.2 Hygro-mechanical properties at the macroscopic scale for different relative humidities

In order to validate the numerical model, different sub-layers that constitute the plant wall have been studied for different behaviors transverse mechanical and hygroscopic. Figure 5 below presents the microfibril angles of the S1, S2 and S3 sublayers as they are respectively −80°, +40°, +60° modelled with ansys.

Figure 6 shows the stress and strain distributions on the fiber at 23% relative humidity obtained by Ansys software while Figure 7 shows the fiber tensile behavior curves at 23%, 54% and 75% relative humidities obtained by simulation in Ansys. It is noticed that whatever the relative humidity the tensile behavior curve presents the same shape. We have a very strong elasticity then, a great ductility before reaching the rupture. This is in accordance with the experimental results presented in the literature which present the RC fiber as having an elasto-ductile behavior [15,18,19,22]. That curve is based on the Hooke's law as presented in equation (1). The same shape is observed on Figure 8 presenting the work that was previously done experimentally on the RC fibers.

From this table we observe a good correlation between the numerical and experimental results for all the mechanical characteristics properties at the different humidities with regard to the variations. As regards the stress at rupture and the elastic modulus, very high values are noted for the experimental tests compared to the results of the numerical simulation. This could be explained by the

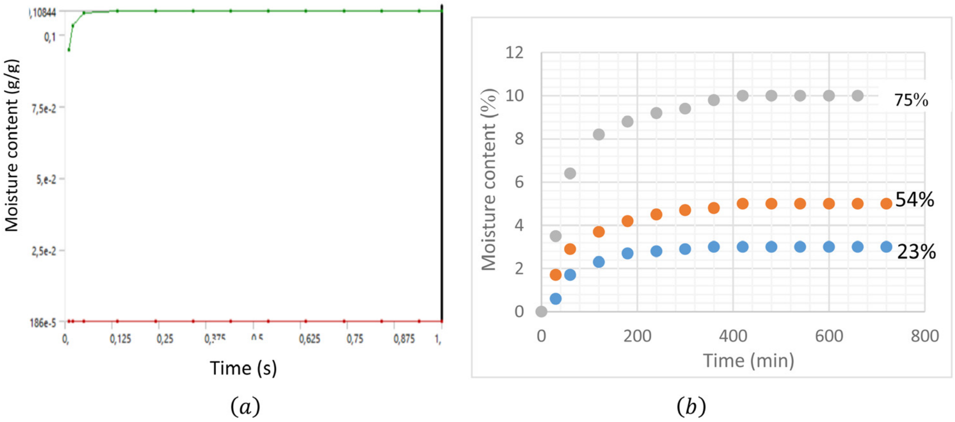


Fig. 3. Adsorption kinetics for an elementary fiber (a) Modeled at a relative humidity of 75% and (b) Experimentally in litterature for 23%, 54% and 75% humidity [17].

Table 5. Water content of RC fiber as a function of RH by the numerical model.

RH	23%	54%	75%	Type
Water content ΔH(g/g)	0,037	0,043	0,108	Numerically
Water content ΔH (g/g)	0,030	0,040	0,100	Experimentally [17]

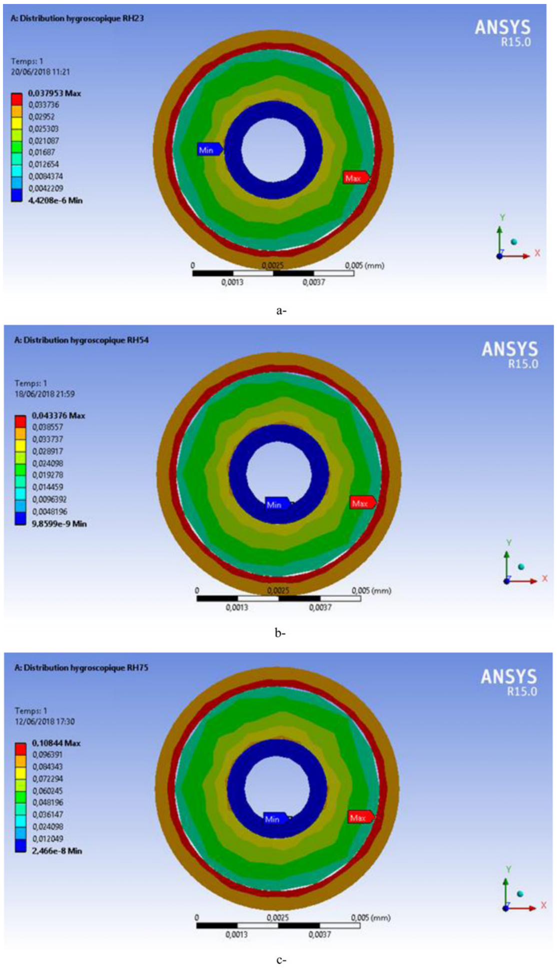
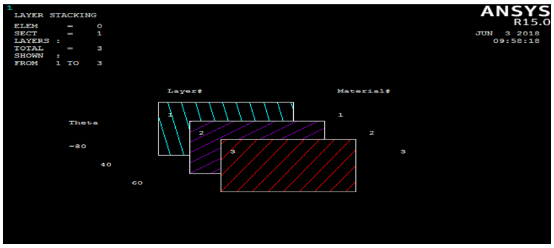


Fig. 4. Hygroscopic distribution within the elementary fiber modeled for the relative humidities of (a) 23, (b) 54 and (c) 75%.



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LAYER STACKING
ELEM      =    0
SECT      =    1
LAYERS :
TOTAL     =    3
SHOWN   :
FROM    1 TO    3
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Fig. 5. Representation of the microfibril angles of the S1, S2 and S3 sublayers on ansys.

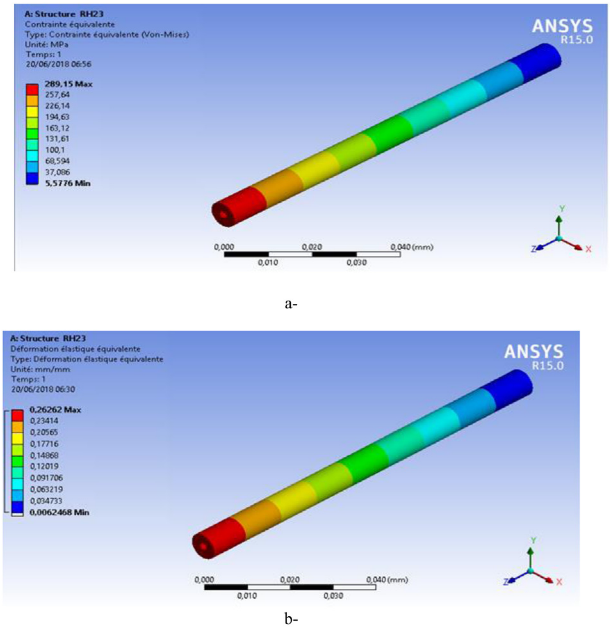

Fig. 6. Distribution on the fiber at a Relative Humidity of 23%: a- stress; b- strain

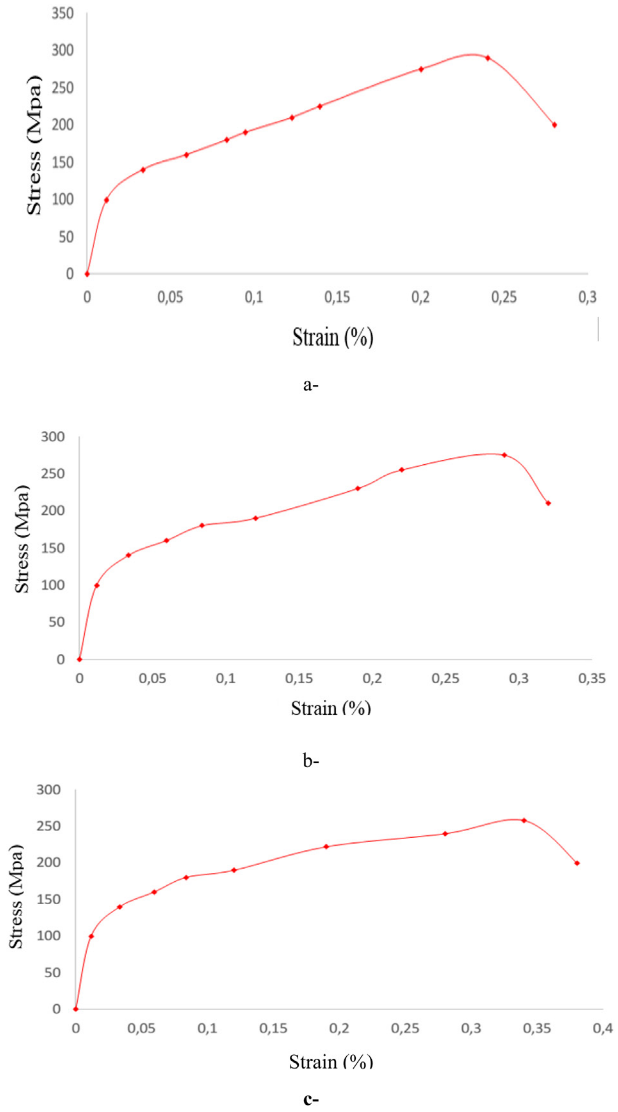

Fig. 7. Model of Tensile behavior curve of the fiber at a relative humidity of (a) 23%; (b) 54% and (c) 75%.

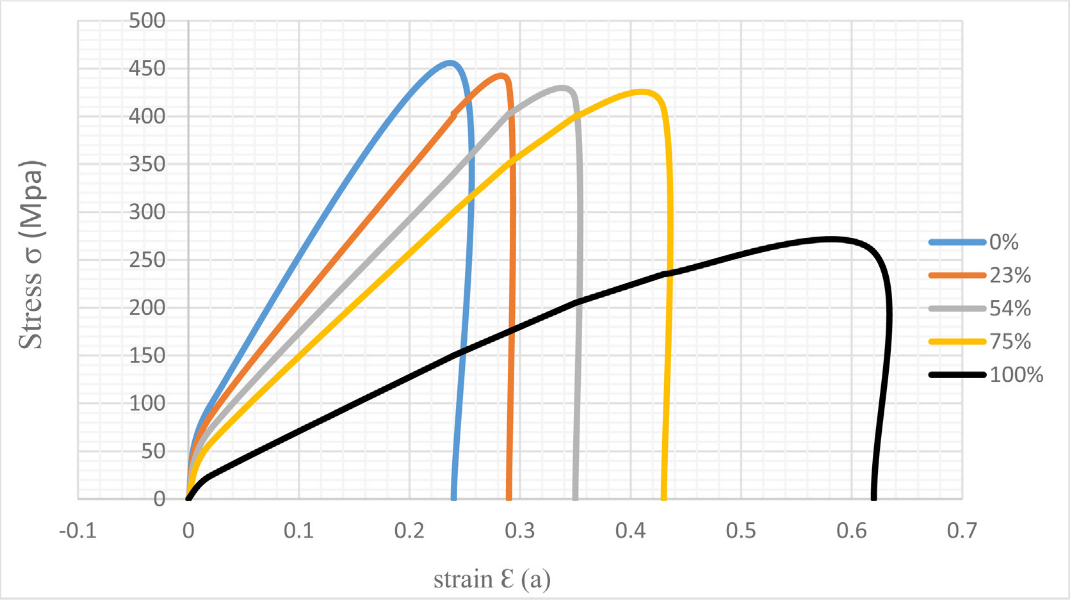

Fig. 8. Tensile behavior of the RC fiber obtained experimentally from litterature [19].

Table 6. Comparison between the tensile behavior of the RC fiber obtained by numerical simulation and experimentally from reference [19].

	Numerical			Experimental [19]			
RH (%)	23	54	75	23	54	75	100
R_m (Mpa)	290	275	259	432.87	416.98	407.11	358.11
A (%)	26	29	34	29.27	35.33	43.32	62.12
E_x (Gpa)	6.4	5.1	3.8	8.66	7.29	5.85	2.43
$\boldsymbol{v}$	0.346	0.328	0.309	–	–	–	–
β_1 (µm/m%)	0.351	0.302	0.299	–	–	–	–

fact that the fibers show quite high dispersion due to harvest location, climate, geometry, extraction, experimental conditions and many others factors. This can also be justified by the fact that many input parameters of RC fiber are not yet known so far and they have been replaced by those of wood which already have a lot of works in that direction. Globally those results are with accordance to the one found in literature concernind others fibers with relative humidities of 30, 40, 50, 60, 70% for flax and nettle [5], flax and sisal [6], flax and Hemp [7], hemp, sisal, flax, jute, agava to the relative humidities of 10%, 25%, 50%, 80% [8] and flax on the relative humidities of 33% and 60% [9] deternined experimentally and flax on the relative humidities of 33% and 60% [9] determined by numerical simulation.

4 Conclusion

Modelling and numerical simulation of hygro-mechanical behavior of Rhecktophyllum Camerunense vegatable fibers using ANSYS sofware were used.. We generally noted that the mechanical properties of RC fibers drop with the moisture as many of the vegetables fibers encounter in the literature and confirm the result got experimentally. The RC fiber remain and elasto-ductile fiber no matter the relative humidity. That bring us to the conclusion that RC fibers should be treated before using them in composite materials to conserve its mechanical properties.

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Conflicts of interest

The authors declare no conflict of interest.

Data availability statement

The authors state the availability of any data at submission.

Author contribution statement

Boris Noutegomo: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Resources, Software, Visualization, Writing – original draft, Writing – review and Editing. Fabien Betene Ebanda: Investigation, Methodology, Project administration, Resources, Supervision, Validation, Visualization, Writing – review and editing. Ateba Atangana: Conceptualization, Formal analysis, Methodology, Project administration, Resources, Supervision, Validation, Visualization, Writing – review and Editing.

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