MULTISCALE STOCHASTIC MODEL AND SIMULATION FOR THE STUDY OF THE NON-LINEAR BEHAVIOUR OF PLANT FIBRE COMPOSITES

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ABSTRACT

In the context of sustainable development, the elaboration and the exploitation of materials and structures requires a minimisation of their environmental impact. In this context, the use of plant fibres for the development of structural composites is a promising solution. Nevertheless, these materials exhibit a relatively complex and non-linear tensile behaviour. Characterisation and understanding of non-linearities, as well as their variability, represent an important challenge for the perennial use of plant fibres as reinforcement of semi-structural composites. This work proposes to investigate the mechanisms that underlie the mechanical behaviour of plant fibre composites using a numerical approach based on a multiscale stochastic modelling. The composite ply is modelled via a representative elementary volume (RVE). The RVE consists of a strand of fibres coated with epoxy matrix. A stochastic method of calculation is implemented. It enables to perform a random drawing of the characteristic parameters of the RVE (dimensional and material) and to carry out a finite elements analysis on the modelled RVE. The preliminary results show that for cylindrical fibres, their dimensions have no influence on the shape of the nonlinear tensile behaviour of the REV of the ply.

1 INTRODUCTION

Plant fibre composites have been booming in recent years in many industrial sectors. While short-fibre and non-woven solutions have reached a good level of maturity, continuous reinforcement solutions are still at a stage of development.

Nevertheless, interesting results have been collected in recent years [1] demonstrating the potential PFCs (Plant Fibre Composites) for semi-structural applications. Several works [2-3] show on the scale of UD (unidirectional) composites a response in non-linear traction.

The origins of this behaviour remain open to discussion in the community.
Several years ago, several hypotheses were proposed that attribute the origin of this non-linear response to mechanisms that occur at different scales (reorientation of cellulose microfibrils or fibres themselves within twisted wires).

Nowadays technological advances make it possible to manufacture, for certain vegetable fibres, tapes and purely unidirectional sheets (i.e. without twists).
In the reinforced composites of such UD structures, a nonlinear response is always observed in [4-5].
These results seem to support the hypothesis that the non-linear behaviour of PFCs results, at least in part, from the non-linear behaviour of plant fibres. Nonlinear behaviour is generally observed at the elementary fibre scale [6]. The work carried out in our team shows that this results from the ultrastructure of the fibre (initial MFA and its possible evolution under mechanical loading [7] and morphological considerations (degree of ellipticity in particular [8]).

This work proposes to investigate the mechanisms that underlie the non-linear behaviour of vegetable fibre composites using a stochastic multi-scale model. The aim is to analyse the mechanical behaviour of a representative elementary volume (REV) of the UD ply (Fig. 1). For this study, the morphological parameters and materials correspond to those of hemp fibres. Nevertheless, the tools and models developed are adaptable to all types of plant fibres.

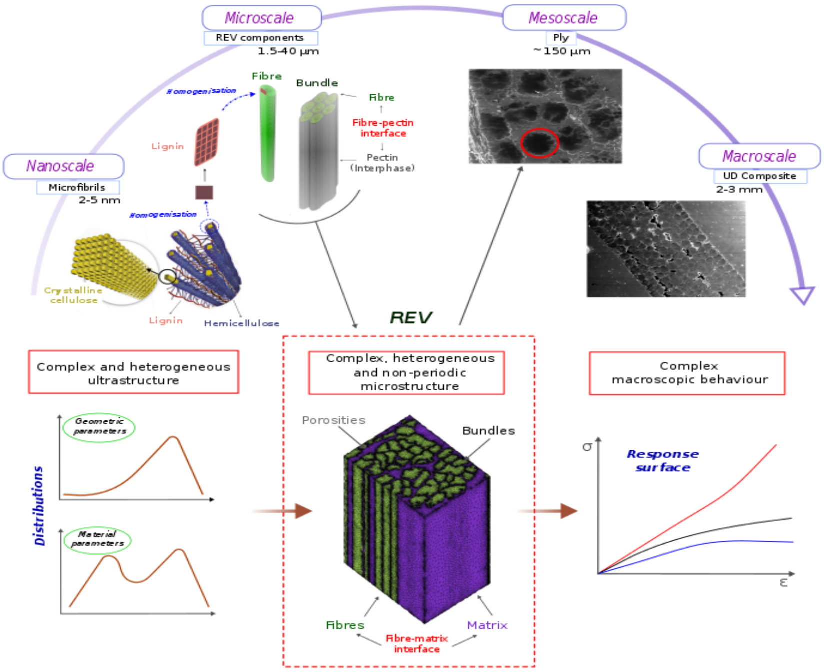

Figure 1: Schematic representation of the multiscale stochastic approach. The model of the REV allows the evaluation of the impact of geometric and material uncertainties occurring at the nano and microscopic levels on tensile behavior at higher scales (meso and macroscopic).

Experimental observations show that the geometry of the fibres is non-uniform and heterogeneous and the distribution of the fibres in the matrix is not periodic. We propose here to consider the strand of fibres impregnated with resin as being the portion of material that can represent the overall behaviour of the ply. The microscopic sections (see Fig. 1) show that the strand consists of individualized individual fibres and bundles of some fibres. We consider here a "perfect" strand, consisting only of perfectly individualized fibres. Within the REV, the fibre wall is considered to be an anisotropic viscoelastic material whose behaviour model is derived from work previously developed in the [7] team. Concerning the stochastic aspects, this work focuses on the variability of the geometric features. Since the morphology of the fibres is very variable, the REV models are generated by expressing the morphological parameters of the fibres by their probability distribution: for each simulation, a set of parameters is defined with a random drawing of these distributions. The models thus parameterized are therefore implemented in a finite element analysis and the tensile test is simulated.

2 METHODS AND MATERIALS

2.1 REV definition

The implementation of a micromechanical approach requires defining a Representative Elementary Volume representative of the material studied. In the literature, several definitions of REV can be found [9].

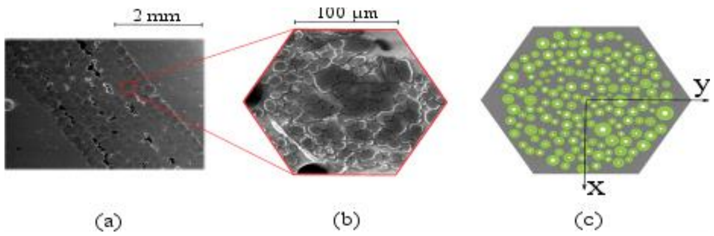

Figure 2: Cross section of an UD fibre composite ply (a), insulated fiber strand (b) and cross section of the geometric model of REV (c).

Nevertheless, they all reveal that the REV should contain enough information about the micro-structure and at the same time be sufficiently small compared to the structural dimensions on the macroscopic scale.

The REV is very clearly defined in only two situations: (i) a unit cell in a periodic micro-structure, and (ii) a volume containing a very large (mathematically infinite) set of micro-scale elements (eg grains), possessing statistically homogeneous and ergodic properties[i] [10].

In the case of UD plant fibre composites, experimental observation shows that the geometry of the fibres is non-uniform and heterogeneous and the distribution of the fibres in the matrix is not periodic. However, a pseudo-periodicity exists between the microscopic scale (elementary fibres, bundles, porosities ...) and mesoscopic (ply) (Fig. 2). Within the ply, the strand of fibres coated in the matrix can be considered as a periodic unit cell.

In this study, we consider that this entity is the REV of the UD ply. A simplified microstructure is chosen as a first step for this REV. The complex morphology of the fibres is simplified and the fibres are modelled as thick-walled cylindrical tubes. The REV is represented by a volume with a hexagonal transverse section containing a sufficient number of fibres, representative of the number observed in an industrially produced strand, and such that the volume fractions of fibre, matrix and porosity measured experimentally are respected.

2.2 Stochastic approach

The stochastic part of this work is expressed in the form of a succession of (deterministic) simulations of models of REV whose parameterization results from a random drawing of the variables, expressed by their probability distribution. For this study, interest is focused only on the geometric variables of the fibres, and in particular on their dimensions.

The method, the flowchart of which is shown in Fig. 3, consists of an initialization step, three main steps and a post-processing step. A Matlab® script controls the various steps, as well as the exchanges between the different software used. All tasks, unless otherwise specified, are performed in the Matlab® environment as well.

Initialization

In this work, a number of input parameters have been set:

- Number of simulations demanded;
- Minimum fibre volume fraction;
- REV geometry (hexagonal section);
- Mesh parameters;
- Behaviour law parameters.

The initialization step allows to set the values for these various parameters.

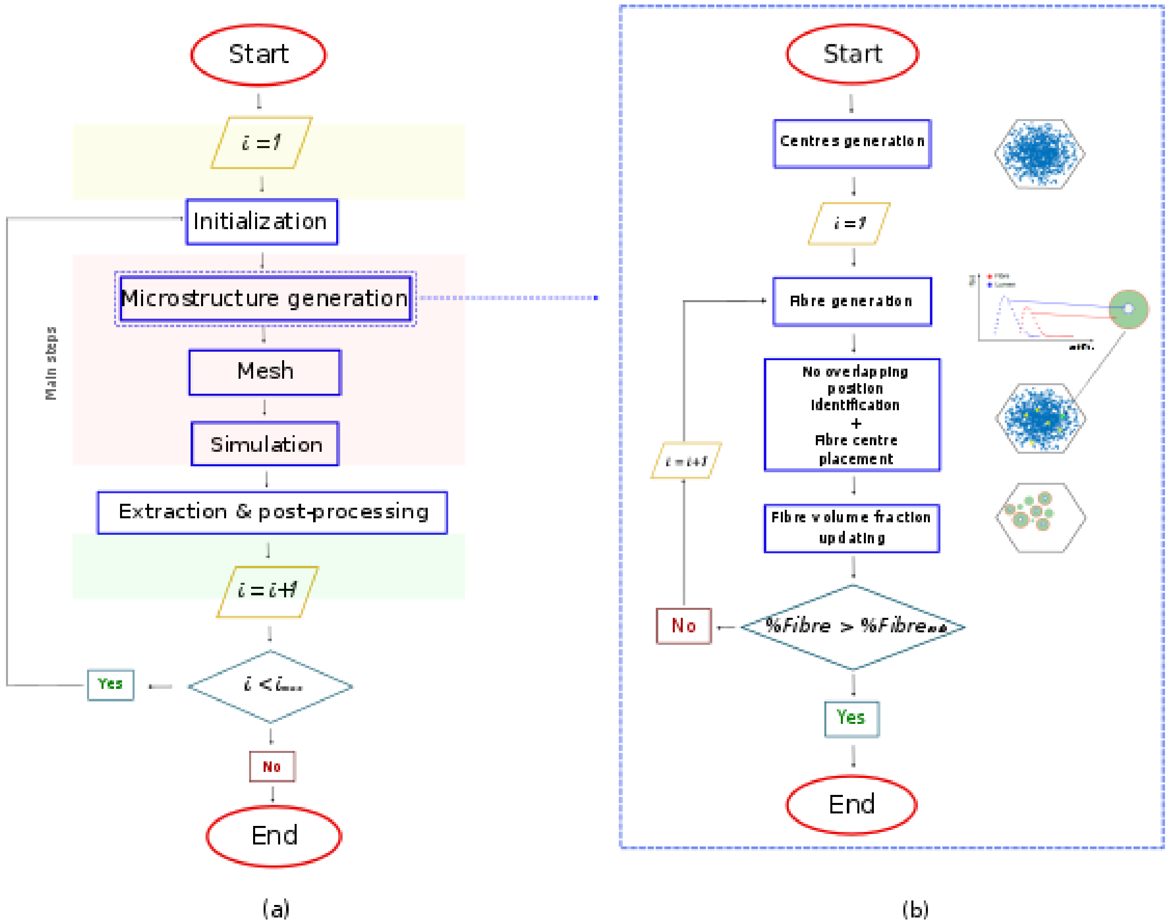

Figure 3: Flow-chart of the analysis phases (a) and detail of the algorithm for fibre generation (b).

STEP 1: Generation of the REV's microstructure

This step consists essentially in generating the microstructure of the REV in the (*x*,*y*) plane. The idea is to generate the fibres and arrange them in the hexagonal section so as to complete the required fibre / matrix ratio. To do this, the algorithm whose flowchart is displayed in Fig. 3b is used. It also consists of three sub-steps:

- Generating possible positions: This initial phase consists of creating a high number of points in the REV section. These points represent the possible positions of the centres of the fibres constituting the strand. The coordinates of these points are created randomly for each simulation carried out in order to keep the randomness of the spatial distribution of the fibres.
- Random drawing of the fibres, one by one: this step allows to define the morphological parameters (diameters) of the fibres composing the REV. For this study, the only parameters considered as stochastic variables are the geometric parameters. Each selection *i* corresponds to a generated fibre.
- Positioning of the fibres: this step of the algorithm allows to place the centre of the fibre generated in the previous step in the section of the REV avoiding the superposition of two or more fibers. The algorithm identifies the points among those generated previously which allows to position the *i*-th fibre without causing overlaps. The generated fibre is randomly centred on one of the identified possible positions. The fibre fraction is therefore updated.

  A test is performed at each iteration until the required fiber volume fraction is reached. The algorithm then continues to position the fibers until there are no more positions available to centre other fibres without overlapping. The geometry is thus validated.

STEP 2: Mesh
Once the section of the REV is completely constituted, the mesh step allows to discretise the geometry and to generate the nodes and the connectivities necessary for the finite elements analysis. The mesh is generated using the free software GMSH [11]. At the output of *STEP 1*, the 2D geometry of the created section is imported into GMSH which performs a surface mesh. This mesh is then extruded in the *z* direction in order to obtain the 3D geometry of the REV.

STEP 3: Simulation
Once the model is created, the tensile test on the REV is simulated using the FE commercial code Abaqus®. The global deformations reached during the simulations are low and the calculations are therefore carried out using an implicit scheme. The calculations are carried out using a quad-core dual processor with 36 GB of RAM.

Post-processing
After each simulation, a python script is executed for the automatic extraction of the results. Once the data is obtained, a Matlab® routine is dedicated to post-processing and storing data. The calculation time for each run and finite element simulation is 2 hours maximum.

2.3 FE model

Solid 8 noded elements are used to model the REV. The fibres are discretized using 20 elements on the outer and inner contours. The REV has 12 elements for each edge of the hexagon and 40 in the height. The conditions of periodicity are imposed by the application of the boundary conditions on the 6 lateral surfaces of the REV (Fig. 4) according to equation:

$$\forall P \in S_i, \quad \vec{u}(P) \cdot \vec{n_i} = 0 \qquad i = [1,6] \tag{1}$$

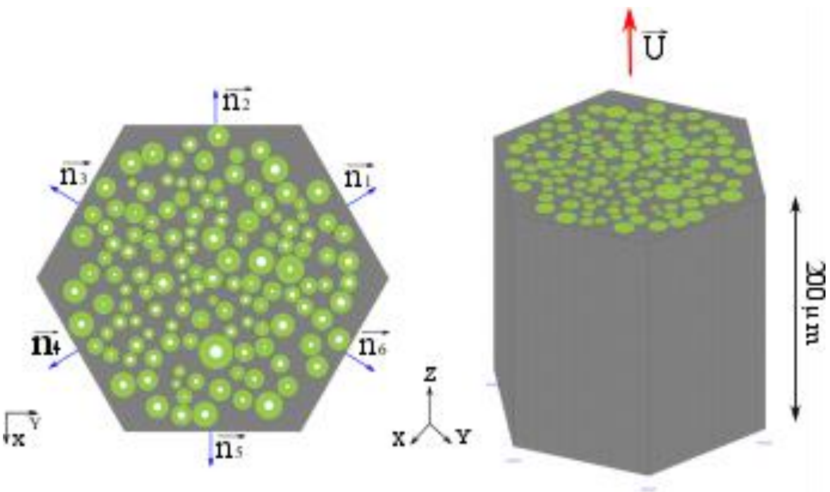

Figure 4: Boundary conditions applied to simulate the tensile test.

The simulations of the tensile test are performed by imposing a nodal displacement at all nodes belonging to the upper surface of the volume. The amplitude of the displacement is chosen in order to impose a deformation rate comparable to that applied experimentally in the quasi-static test, i.e. $\dot{\varepsilon} = 10^{-4}s^{-1}$. The simulated maximum global deformation is equal to 2%. The bottom surface is embedded to prevent rigid body movements. The global stress is obtained as the ratio between the sum of the reactions to the imposed nodal displacements and the surface area of the REV. This surface is calculated by taking into account the porosities (lumens) and neglecting the variations which during the tensile test.

2.4 Behaviour law

Fibre wall

For this study, an anisotropic viscoelastic behavior is implemented to model the behaviour of fibres. The wall of the fibres is considered as a composite material in which the reinforcement and the matrix are respectively represented by the cellulose microfibrils and by a mixture of hemicellulose and lignin. The elastic properties are calculated by homogenization [12], the viscoelastic parameters were previously identified by inverse method using creep tests performed on elementary fibres [13, 14]. The model is described in detail in Trivaudey et al. [7]. The parameters used, elastic and viscoelastic, are summarized in Table 1. In this study, the reorientation of microfibrils in the fibre wall during the tensile test is taken into account, with an initial angle (MFA) equal to 11 ° for all the fibres.

Elastic properties		Viscoelastic parameters	
E_L	75 GPa	β_{LT}	12.25
E_T	11 GPa	β_T	1.5
ν_{LT}	0.153	zn_c	2.45
G_{LT}	2.52 GPa	zn_0	1.9
ν_{TT}	0.2		–

Table 1: Elastic and viscoelastic parameters used to feed the fibre behavior model. Directions L and T correspond to the longitudinal and transverse directions in the local reference frame linked to the microfibrils [7].

Matrix

Concerning the matrix, in this work, its behaviour is considered purely elastic, with E = 4 GPa and ν=0.34. The damaged and plastic behaviour will be taken into account in a future work.

The porosities taken into account in this work correspond to the total volume of voids (lumen) in the REV. These areas are considered to have zero rigidity. The porosities generated during the manufacturing process of the composite, within the matrix, are not taken into account in this first version of the work.

3 RESULTS

3.1 Characterization of the generated microstructures

A first sequence of 100 simulations is carried out to evaluate the impact of the geometric parameters on the behaviour of the REV. To do this, the diameters of the fibres and the lumens are drawn randomly from the probability distributions of the measurements of the areas. The parameters of the probability laws are summarized in Table 2.

	Fibre surface [μm^2]	Lumen surface [μm^2]
Distribution law	*Lognormal*	*Lognormal*
μ	*6.9365*	4.3371
σ	0.4734	0.8304
Maximum error on the generated distributions		
Err(μ)	*0.121%*	0.332%
Err(σ)	0.072%	0.008%

Table 2: Parameters of estimated probability laws on measurements of hemp fibres and lumens surfaces. Difference on the parameters of distribution laws estimated on the generated VER compared to the experimental ones.

Since the generation process of the REV microstructure is random, an analysis of the geometrical characteristics of the REVs obtained is carried out.

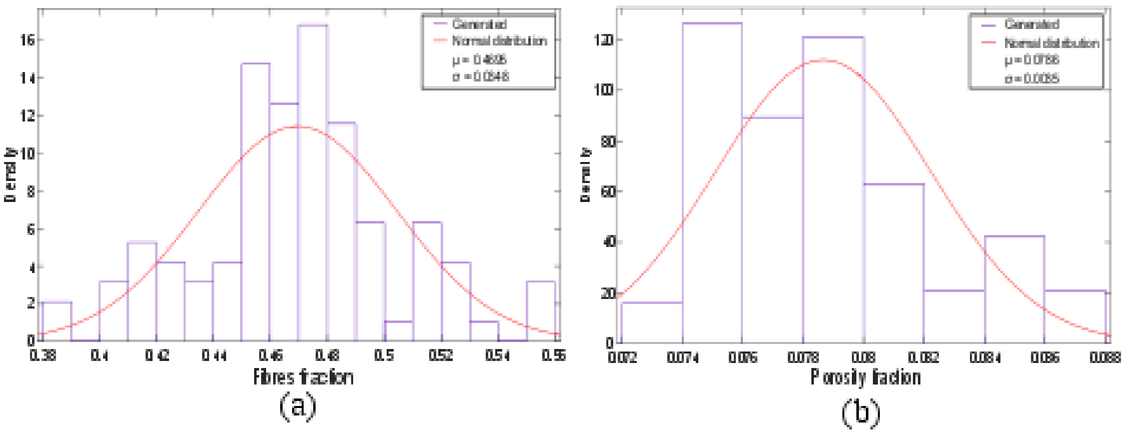

Figure 5: Probability distributions of the fibres (a) and the porosity fractions (b) obtained.

For each REV generated, the probability distributions of the surfaces of the fibres and the lumens are in agreement with those resulting from the experimental observation. The differences between the parameters of the generated probability and experimental laws are shown in Table 2. The REV generation method is therefore capable of reproducing efficiently and automatically the elementary volumes of which the geometrical characteristics agree with the data obtained experimentally. As described previously, the REV generation algorithm takes as input the morphological parameters of the fibres in the form of probability distributions, the size of the elementary volume and a minimum volume fraction of fibers required. The volume fraction obtained, as well as the porosity rate, result from the random drawing carried out for the dimensions of the fibres, but also for the positions of the centres. The probability distributions of the fiber fractions and the porosity rates obtained for the simulated REVs are shown in Fig. 5. The volume fraction of fibres varies in the REV, for the simulations considered, from 38% to 55%. The porosity rate is between 7% and 8.8% of the total volume.

3.2 Tensile test simulation: comparison with the literature

The Fig. 6 proposes a stress-strain curve obtained by numerical simulation of a tensile test on a REV containing a hundred elementary fibers impregnated in the epoxy resin. The generated microstructure has a fibre volume fraction of 38%. In this figure, some experimental curves extracted from the literature are also reported. They concern lin-epoxy [15] and jute-polyester composites [5], failing to be able to present results for hemp-epoxy UDs. This first result shows that the stress levels obtained with the REV model used here are comparable to those observed experimentally for similar materials.

The shape of the curve is also close to that observed experimentally for these PFCs. Nevertheless, it is possible to note that the yield point observed experimentally around 0.2% deformation is not reproduced by numerical simulation. The origin of this non-linearity observed experimentally is probably due to physical mechanisms not taken into account in our model, such as dissipative phenomena (damage and / or plasticity) that can occur within this type of composite. Consideration of these mechanisms is envisaged in the rest of this work, and the influence of the parameters of the behavior law on the response of the ply will be quantified.

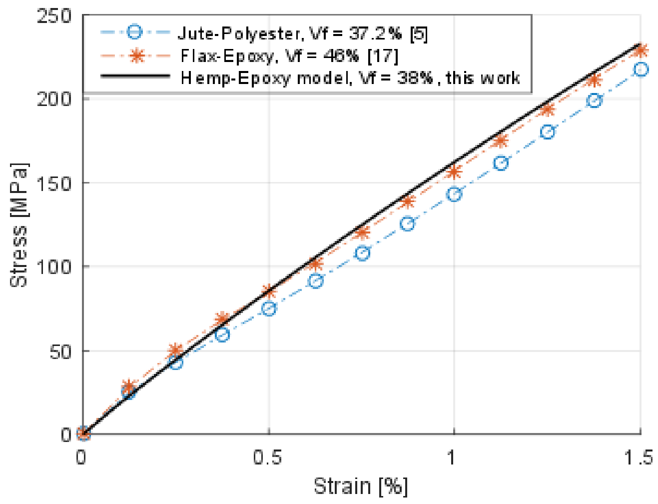

Figure 6: Comparison of the tensile behavior of various UD plant fibre composites reported in the literature from tests and simulations carried out from the representative volume of a hemp-epoxy ply presented in this study.

3.3 Tensile test simulation: influence of the geometric features

The results of the simulations obtained for the 100 REVs tested are presented in Fig. 7. Observing the results obtained, we note that all the microstructures studied express the same type of tensile behaviour and non-linearity.

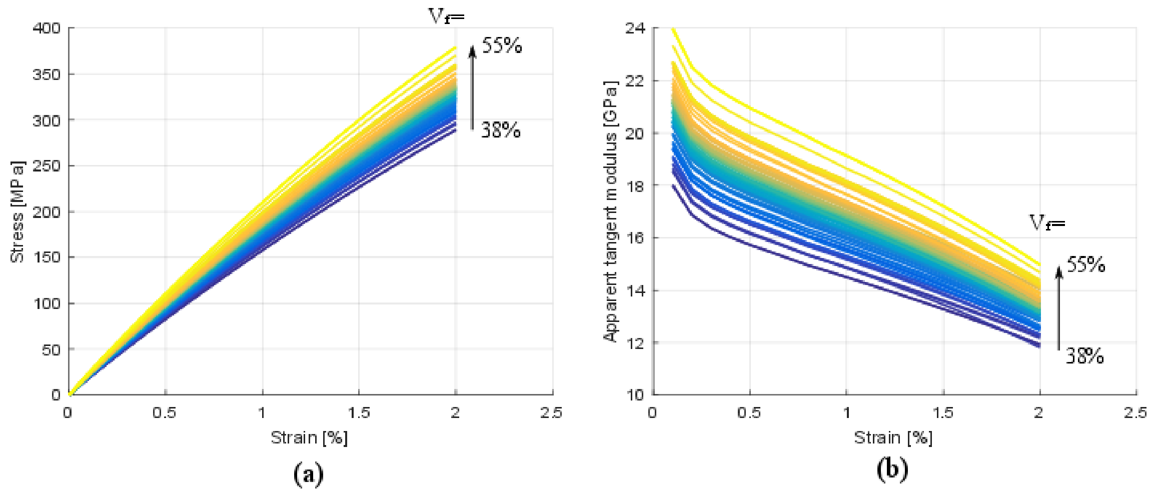

Figure 7: REV global tensile behavior with microstructures with variable fibre sizes (a). Apparent tangent moduli curves (b).

The apparent tangent modulus decreases as the axial deformation increases. Differences are observed, particularly with regard to rigidities. These appear to be advantageous because of the volume fraction of fibres, rather than the size or distribution of the fibers themselves. Indeed, at this stage of the work it is difficult to distinguish the effects of fibre size (or fibre size distribution) on the effect of the volume fraction of fibres, since the random draws made to construct the microstructures not only lead to a modification of the size and distribution of the fibres in the REV, but also to the fibres volume fraction. By determining the volume fraction of each of the REVs tested, and as expected, it appears that the highest rigidities are obtained for the microstructures which lead to the highest fibre content.

Calculations are under way on microstructures with variable fibre size and distribution but identical volume fraction. These results will consolidate the previous conclusion.

4 CONCLUSIONS

This study presents a methodology for the analysis of the mechanical behaviour of plant fibre composites based on a multi-scale stochastic approach. The composite ply is represented by an elementary volume consisting of a strand of fibers embedded in an epoxy matrix. The microstructures of the REVs are generated automatically using random draws within the distribution laws of the geometrical parameters of hemp fibres. The results obtained from a first series of simulations show that:

- The geometrical characteristics of the generated REV microstructures respect the distributions obtained from experimental observation;
- The shape of the non-linearity remains the same for all simulated REVs.
- The apparent stiffness of the ply seems independent of the size and distribution of the fibres within the REV, at least when the latter have a circular transverse section;

These are only preliminary results, and they do not allow to decouple the influence of the fibres volume fraction and that of the geometrical parameters of the microstructure. In the future works, the REV generation method will be exploited in order to carry out a sensitivity analysis on the geometrical and morphological parameters on the tensile behavior of the REVs.

In the next steps, REVs with constant volume fraction with different microstructures will be simulated. The idea will be to vary the fibre dimensions in the REV, as well as their morphology, to finally evaluate the propagation of the geometric effects observed for the elementary fibers [8] on the scale of the UD reinforcement.

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[i] For a stationary random process, it is assumed that the statistical characteristics derived from the mean values calculated from the values at the same instant of a large number of different realizations of the process in question coincide with those which are deduced from the successive values in time of any of these realizations