A multiscale model-based investigation of the non-linear tensile behaviour of plant fibre composites

A. Del Masto[1], F. Trivaudey[1], V. Guicheret-Retel[1], V. Placet [1]

[1] *Univ. Bourgogne Franche-Comté, FEMTO-ST Institute, CNRS/UFC/ENSMM/UTBM, Department of Applied Mechanics, 25000 Besançon, France*

Abstract

Unidirectional plant fibres reinforced composites (UD PFRCs) are complex, hetorogeneous and hierarchical materials and represent the most interesting family of biobased camposites for structural high-performance applications. Experimental studies pointed out that UD PFRCs show a nonlinear tensile behaviour when loaded in the reinforcement direction, along with a slight variability in their mechanical properties. The origins of this particular mechanical response are still open to discussion. In this study we propose to numerically assess the impact of material and morphological parameters belonging to the nano, micro and mesoscales of the UD composite on the apparent stiffness of the single ply through sensitivity analysis. A multiscale-stochastic approach is developped through the definition of a parametric Representative Volume Element (RVE) of the UD ply, comprised of a unidirectional roving of about 100 individualised fibres embedded in an epoxy matrix. Results of polynomial chaos expansion based sensitivity analysis allow the identification of the most influential parameters on the stiffness of the ply, which are the longitudinal modulus of the crystalline cellulose, the fraction of cellulose and the initial microfibrillar angle.

Keywords: Plant fibre composites, FEM, RVE, Multiscale-stochastic approach, Sensitivity analysis

1 Introduction

Ecological and economical issues prompt an increasing number of industrial and academic researchers to focus on high-performance materials that comply with all the new environmental preservation interests. Natural fibres are good candidates for replacing synthetic man-made fibres in reinforcing organic matrices in high-performance composite applications [1]. Two major diffculties lie with the use of plant fibres composites (PFCs): (*i*) their nonlinear mechanical behaviour and (*ii*) the variability of their mechanical properties and behaviour [2]. The mechanisms responsible of this particular response are not yet well understood. Nonlinearity and variability are also generally observed at the lower scale of the elementary fibres [3]. These results seem to support the hypothesis that the nonlinear behaviour of PFRCs may result, at least in part, from the nonlinear behaviour of the single fibres themselves. And since the tensile behaviour of fibres depends on their morphology, ultrastructure and material properties of biopolymer constituents of the fibre wall at the nanoscale, these features may affect the mechanical response at the higher scales of the composite too.

This study is dedicated to the assessment of the impact of several morphological and material parameters belonging to different scales on the tensile stiffness of the UD biobased composite using a multiscale stochastic approach. The mechanical behaviour is investigated at the scale of an elementary volume, assumed to be representative of the UD ply. This Representative Volume Element (RVE) is made of a non-twisted roving of about 100 individualised fibres embedded in an epoxy resin, modelled considering a perfectly elastic behaviour. Within the RVE, the fibre morphology is simplified (circular and elliptical shape of the transverse section) and the fibre wall is considered to be an anisotropic viscoelastic material of which behaviour model is derived from work previously developed in our team [4]. The stochastic aspect of the proposed approach is expressed through a succession of deterministic FE simulations made at the scale of RVE with randomly generated microstructures, each one representing an outcome of the probability distribution functions (PDF) of material and morphological parameters experimentally observed at nano, micro and mesoscale within the RVE itself. The behaviour of all generated RVEs is then evaluated through a FEM simulation of the tensile test. The developed approach is used to assess the impact of the mean values of some morphological and material parameters' PDFs within the RVE on its tensile properties through a polynomial chaos expansion based sensitivity analysis [5].

2 Methods and materials

2.1 Multiscale-stochastic approach

In order to implement the proposed approach, a software tool is developed. For each simulation, five steps succed one other:

1) The analysis is initialised and the PDFs of each marphological and material parameter considered are setted from means and standard deviations randomly drawn from the experimental ones proposed in the literature (flax fibres);
2) The RVE two-dimensional microstructure is generated adding one fibre at the time. The geometrical and material properties of the constituents at the nanoscale of the wall affected to each fibre are randomly drawn from the PDFs determined at the first step. The fibres are embedded in a elastic epoxy matrix, modelled as a isotropic perfectly elastic material ($E = 4GPa$ and $\nu = 0.3$). The interphases between fibres and matrix are modelled as a thin layer expressing an isotropic elastic behaviour ($E = 1GPa$ and $\nu = 0.3$);
3) The generated microstructure is meshed in 2D using a combination of Matlab® code and free mesh generator Gmsh. The 2D mesh is and then extruded in the third dimension to obtain the 3D model of the impregnated yarn;
4) A simulation of the tensile test is carried out on the generated 3D model using the FE code Abaqus®;
5) The results of the simulation are post-processed using Python and Matlab® codes in order to obtain the global tensile behaviour of the simulated RVE.

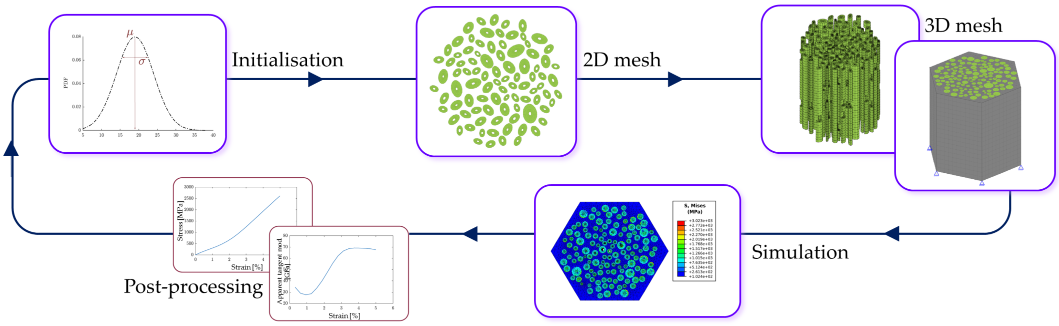

Figure 1: *Multiscale-stochastic approach*

2.2 Polynomial chaos expansion-based sensitivity analysis

The developed multiscale-stochastic approach is used to represent the RVE's apparent tangent modulus at the beginning of the loading on a polynomial chaos basis. The observed output $\mathbf{Y}$ can be expressed as $\mathbf{Y} = \sum_{\alpha \in \mathbb{N}^\mathbf{k}} y_\alpha \Psi_\alpha(\mathbf{X})$, where y_α represent the coefficients of the polynomial chaos expansion, $\Psi(\mathbf{X})$ are multidimensional polynomes of degree $|\alpha| = \sum \alpha_i$ and k is the number of input parameters. The y_α coefficients are computed using a regression method and then used to compute the sensitivity indices, *i.e.* to estimate the impact on the observed output, of the considered morphological and material parameters. Two families of indices are computed: first order, which assess the linear effect of the i^{th} parameter on the observed output, and total index, which estimate the global impact of the i^{th} parameter, including the effect of interactions with other variables:

$$S_i, S_{Ti} = \sum_{\alpha \in \mathcal{A}_i} \frac{y_\alpha^2}{\mathcal{D}} \quad \text{for} \quad \begin{cases} \mathcal{A}_i = \{\alpha \in \mathbb{N}^k : \alpha_i > 0, \alpha_{j \neq i} = 0\} \rightarrow S_i \\ \mathcal{A}_i = \{\alpha \in \mathbb{N}^k : \alpha_i > 0\} \rightarrow S_{Ti} \end{cases} \tag{1}$$

where $\mathcal{D}$ represents the variance of the observed output. Five parameters are considered, both material and morphological, which have been previously identified using a grouped screening analysis as the most influential on the apparent stiffness of the RVE: longitudinal modulus of crystalline cellulose $E_{L_{cc}}$, fraction of cellulose m_c, initial microfibrillar angle ψ, fibre D and lumen d diameter. It's worth notice that among the previously identified most influential variables there are, quite surprisingly, two morphological parameters (D and d) alongside the expected material ones ($E_{L_{cc}}$, m_c, ψ).

3 Results

The results in terms of first order and total sensitivity indices are shown in figure below. The computed sensitivity indices shows that three parameters have the greatest impact on the initial apparent stiffness of the UD ply: the longitudinal modulus of crystalline cellulose $E_{L_{cc}}$, the fraction of cellulose m_c and the initial microfibrillar angle ψ.

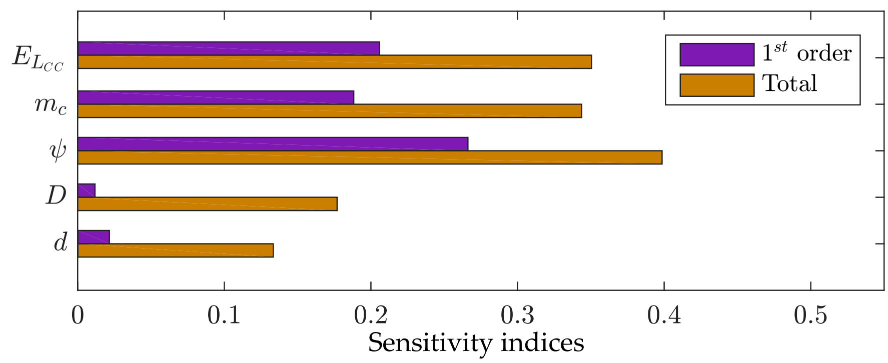

Figure 2: *Sensitivity indices computed through polynomial chaos expansion*

4 Conclusions

A stochastic-multiscale numerical approach is developped in order to explore the origins of the nonlinear behaviour of UD PFRCs. The composite ply is represented by an elementary volume consisting of a roving of flax fibres embedded in an epoxy matrix. The microstructures of the RVEs are generated automatically using random draws from the probability distribution functions of morphological an material parameters belonging to different material scales.

The proposed approach is applied to a polynomial chaos expansion-based sensitivity analysis, in order to assess the impact the considered parameters on the apparent initial stiffness of the UD ply. Results show that the most influential parameters on the stiffness of the UD ply are the longitudinal modulus of crystalline cellulose $E_{L_{cc}}$, the fraction of cellulose m_c and the initial microfibrillar angle ψ. This study allows a first evaluation of the propagation of the mechanical behaviour through the characteristic material scales of UD biobased composites. The next step will be to model more complex morphologies of fibres and to include in the analysis irreversible phenomena, like plasticity and damage, in order to evaluate the impact of morphological and material parameters on the rupture behaviour of the ply.

References

[1] A. Bourmaud, J. Beaugrand, D. U. Shah, V. Placet, C. Baley, *Towards the design of high-performance plant fibre composites.* Progress in Materials Science, 97, pp. 347-408, 2018.

[2] D. U. Shah, *Damage in biocomposites: Stiffness evolution of aligned plant fibre composites during monotonic and cyclic fatigue loading.* Composites Part A: Applied Science and Manufacturing, 83, pp. 160-168, 2016.

[3] V. Placet, O. Cissé, M. Lamine Boubakar, *Nonlinear tensile behaviour of elementary hemp fibres. Part I: Investigation of the possible origins using repeated progressive loading with in situ microscopic observations.* Composites Part A: Applied Science and Manufacturing, 56, 319-327, 2014.

[4] F. Trivaudey, V. Placet, V. Guicheret-Retel, M. Lamine Boubakar, *Nonlinear tensile behaviour of elementary hemp fibres. Part II: Modelling using an anisotropic viscoelastic constitutive law in a material rotating frame.* Composites Part A: Applied Science and Manufacturing, 68, 346-355, 2015.

[5] B. Sudret, *Global sensitivity analysis using polynomial chaos expansions*, Reliability Engineering and System Safety, 93, pp. 964-979, 2008.