



Nonlinear tensile behaviour of elementary hemp fibres. Part II: Modelling using an anisotropic viscoelastic constitutive law in a material rotating frame



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ABSTRACT

A 3D viscoelastic model is presented, based on the use of finite element method for the study of the nonlinear tensile behaviour of hemp fibres. On the basis of an experimental investigation, Part I of this study (Placet et al., 2014) proposed a scenario based on several physical mechanisms, in order to explain the nonlinear behaviour of such fibres. These mechanisms included viscoelastic strain, cellulose microfibril reorientation, and shear strain-induced crystallisation of the amorphous paracrystalline components. The second part of this ongoing study proposes to implement such mechanisms and the associated constitutive laws in a simplified 3D model, in order to evaluate the contribution of each mechanism to the macroscopic tensile behaviour of the fibre.

The results show that the proposed anisotropic viscoelastic constitutive law, describing finite transformations through a material rotating frame formulation, is able to accurately simulate the shape of the experimentally observed tensile curves. This model is also used to investigate the influence of dislocation areas on the tensile behaviour and stress fields.

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1. Introduction

Cellulose fibres from wood and plants represent a promising class of reinforcement materials, for use in high-performance polymer matrix composites. Because natural fibres are characterised by the strong variability of their mechanical properties and their high sensitivity to temperature and humidity, the design of reliable structure-based composites containing such natural fibres is a significant challenge for engineers, who are accustomed to using the consistent and accurate data available in the case of man-made fibres. These last ones are inherently produced in highly-controlled conditions, unlike natural fibres.

In addition to their highly scattered mechanical properties, numerous fibres are characterised by nonlinear tensile behaviour. The understanding of this particular behaviour is of great importance, in view of the development of composites reinforced with plant fibres, since the behaviour of these fibres could have an

impact on their performance when they are used to reinforce composite materials. Several authors have recently observed nonlinear behaviour in unidirectional composites reinforced with flax fibres [1–5]. Some authors have also mentioned an increase in stiffness under cyclic loading, a behaviour which has been observed at the scale of individual fibres [6].

Many hypotheses have been proposed in the literature to explain the nonlinear tensile behaviour of isolated wood or plant fibres, and the fibres' stiffness recovery or improvement after loading beyond the yield point. These hypotheses were discussed in Part I of this study [7]. In the case of wood tracheids, Page et al. [8] confirmed a relationship between the nonlinear shape of the tensile curve and the onset of cell wall buckling. They clearly showed that the yield point (i_1) corresponds to the onset of wall buckling. More recently, Eder et al. [9] also showed that thick-walled fibres are highly resistant to tension buckling, and that this phenomenon can therefore explain the nonlinearity of the stress–strain curve only, in the case of a thin-walled fibre. Since hemp fibres generally have a thick wall, tension buckling therefore does not explain the nonlinearity of the stress–strain curve in the case of such fibres. Other authors have also attributed nonlinear behaviour to irreversible reorientations of the cellulose microfibrils with respect to the fibre axis in particular in the S_2 layer, when they

Abbreviations: C, crystallisation; D, default; E, elastic behaviour; MFA, cellulose microfibrils angle; MFR, cellulose microfibrils reorientation; VE, viscoelastic behaviour.

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Nomenclature

$(\vec{X}, \vec{Y}, \vec{Z})$	global coordinate system related to the fibre (Z: axial direction)	μ_i	weighing coefficients of the viscous mechanisms
		τ_i	release times of the viscous mechanisms
		$zn_c, 0, \Delta$	shape parameters of triangular spectrum distribution of the relaxation times (centre, half-width, interval between two relaxation times)
<i>Mechanical tensors</i>		σ_0	constant axial stress.
$\underline{\sigma}$	Cauchy true stress tensor	$J_{ZZ,mod}^k(t)$	computed axial viscoelastic compliance function
$\underline{\varepsilon}$	total strain tensor	$J_{ZZ,exp}^k(t)$	experimental axial viscoelastic compliance function
$\underline{\varepsilon}^e$	elastic strain tensor	$J_{ZZ,mod}^k(k \in \mathbb{N})$	kth computed value of axial viscoelastic compliance
$\underline{\varepsilon}^{ve}$	viscoelastic strain tensor	$J_{ZZ,exp}^k$	k th value of the experimental axial compliance data
\underline{S}	elastic compliance tensor	<i>Transformation</i>	
\underline{S}^{ve}	viscoelastic compliance tensor	\underline{F}	deformation gradient
<i>Elastic parameters</i>		ψ	supplementary angle of the microfibrils angle
$E_L, E_T, \nu_{LT}, \nu_{TT}, G_{LT}$	layer elastic properties (longitudinal and transverse moduli, Poisson's ratios, and shear modulus)	$\tilde{\chi}^0$	microfibrils direction prior to transformation
<i>Viscoelastic parameters</i>		$\tilde{\chi}$	microfibrils direction after transformation
$\beta_T, \beta_{TK}, \beta_{LT}$	parameters characterising the layer viscosity	Q_f	rotation tensor
$\underline{\tilde{s}}_i (i \in \mathbb{N})$	second order tensors corresponding to elementary mechanisms of viscoelastic flow	$(\vec{e}_{01}, \vec{e}_{02}, \vec{e}_{03})$	Lagrangian frame
		$(\vec{e}_1, \vec{e}_2, \vec{e}_3)$	material frame

are submitted to axial loading. S_2 is the main sub-layer of the cell wall in terms of its thickness and therefore contributes mainly to the global mechanical behaviour of the fibre. A linear fit was established between the microfibril angle (MFA) and strain for coir fibres, by Martinschitz et al. [10]. Other authors have attributed this nonlinear behaviour to shear deformations in the non-crystalline region, which can partially damage the cell wall, or provoke a stick-slip phenomenon [11]. This stick-slip mechanism proposed by Keckes et al. [11] operates like a 'molecular Velcro'. According to these authors, beyond the yield point (i_1) the shear stress could provoke a viscous flow of the matrix. When the stress is released there would be no back-flow of the matrix, but a lock-in phenomenon associated with immediate bond re-formation in the fibrils' new position. This could explain irreversible strain without significant damage. This model supposes the presence of non-covalent interactions between hemicellulose chains attached to adjacent cellulose microfibrils. Altaner and Jarvis [12] proposed an alternative model in which hemicellulose chains bridging continuously from one microfibril aggregate to the next. However, the mechanism is different; the computed tensile curves are similar to those of the original model.

Nonlinear tensile behaviour was modelled by Nilsson and Gustafsson [13] for hemp fibres, by introducing defects into the helical structure of the cellulose microfibrils and assuming that the hemicellulose has an elasto-plastic constitutive relation. Navi and Sedighi-Gilani [14,15] proposed a model for wood fibres with an elasto-plastic behaviour for amorphous polymers, based on the assumption of a helical, non-uniform distribution of cellulose microfibrils in the fibre and damage to the amorphous constituents after yielding. The origin of the dissipative behaviour of elementary fibres is thus attributed to plasticity by these authors.

In the Part I of this study, using experimental investigations we proposed a scenario centred on several physical and microstructural mechanisms, in order to explain the nonlinear behaviour (type 3) of such fibres, including viscoelastic strain, cellulose microfibril reorientation and shear strain-induced crystallisation of the amorphous cellulose. In the present, second part of the study, we propose to implement such mechanisms, together with the associated constitutive laws, into a 3D model which can be used to evaluate the contribution of each physical mechanism to the macroscopic tensile behaviour of type 3of the fibre.

2. Modelling

2.1. 3D model

The macroscopic simplified 3D model used for this study is based on a previously developed model, described in detail in [16]. The elementary hemp fibre is idealised as a single-layered, hollow, thick-walled cylinder made of an orthotropic material having a helical orientation (corresponding to the cellulose microfibril orientation). The possible variation in cross-section shape and size along the fibre length, non-unity transverse aspect ratios (i.e. non-circular cross-section) and their induced effects on the fibre mechanical behaviour (stress concentration, fibre rotation...) are therefore not addressed in the model. The transverse anisotropy introduced by non-unity aspect ratios is also in consequence ignored in this model. The wall is modelled as if it were a long fibre-reinforced composite material, made with a mixture of three different polymers. The wall properties are determined using a homogenisation technique [16]. The values obtained for its elastic properties are summarised in Table 1. The fibres were considered to be free to rotate, and the influence of the boundary conditions on the computed value of the apparent modulus was studied in Part I of this paper. It was shown that although the testing device prevented the fibre from rotating during tensile tests, the experimentally determined value of the apparent E-modulus was more closely related to the numerical value determined using a free rotation. This was explained by the relatively strong hypothesis of cellulose microfibril continuity formulated when constructing the model.

Hygro-mechanical coupling was not considered in this version of the model.

Table 1
Values of the model parameters used in the FE computations.

Elastic parameters		Viscoelastic parameters	
E_L	75,000 MPa	β_{LT}	12.25
E_T	11,000 MPa	β_T	1.5
ν_{LT}	0.153	zn_c	2.45
G_{LT}	2 520 MPa	zn_0	1.9
ν_{TT}	0.2		

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