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Predicting hygro-elastic properties of paper sheets based on an idealized model of the underlying fibrous network

Emanuela Bosco [a,b,*], Ron H.J. Peerlings [b], Marc G.D. Geers [b]

[a] Materials innovation institute (M2i), P.O. Box 5008, 2600 GA Delft, The Netherlands
[b] Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

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ABSTRACT

Significant dimensional variations may occur in paper-based materials when subjected to changes in moisture content. Moisture induced deformations are governed by the swelling of individual fibres, which is transferred through inter-fibre bonds to the entire fibrous network. Complex interactions between mechanical and hygro-expansive properties take place in the bonding areas, affecting the overall material response. In most network models, the role of these inter-fibre bonds is not explicitly incorporated. This work presents a periodic meso-structural model for the discrete fibrous network, which considers the free-standing fibre segments *and* inter-fibre bonds. Despite its simplicity, the reference unit-cell enables the incorporation of relevant micro- and meso-structural features such as network structure, fibres and bond geometry and hygro-elastic properties. The proposed model is solved analytically through a proper homogenization strategy, allowing to recover the paper's anisotropic hygro-mechanical response in terms of effective elastic constants and effective hygro-expansive coefficients, exploiting the coupling at the meso-structural level between hygroscopic and mechanical behavior. A comparison with experimental results obtained from the literature shows that the presented approach is quite accurate in predicting the overall paper response, thereby revealing the influence of several meso-scale parameters (e.g. fibre orientation, dimensions, mechanical strength).

1. Introduction

Paper is a material consisting of cellulose fibres bonded to each other to form a discrete network (Niskanen, 1998). Due to the production process, fibres have a preferential orientation along the direction of manufacturing, resulting in a significant anisotropy of the material. A distinctive feature of paper is its sensitivity to changes in moisture content, which lead to pronounced dimensional variations at different length scales. The hygro-expansive response of paper originates at the fibre level, where a single fibre exhibits strongly anisotropic moisture induced deformations. The fibres' hygro-expansive behavior is transferred within the meso-structural network through the inter-fibre bonds, where micro-stresses generally appear due to the interaction between mechanical and hygro-expansive properties of the fibres (Larsson and Wagberg, 2008). All of these phenomena in the underlying fibrous structure concur to yield the overall moisture induced deformations at the sheet level, which can be represented with reasonable approximation through a linear relation with respect to the humidity variation (Nanri and Uesaka, 1993). Hygro-expansive strains significantly influence the industrial performance of the material, for instance in relation to the runnability during printing operations. Understanding how the effective properties of paper are controlled by the hygro-mechanical response of individual fibres and the fibrous network is thus highly relevant for industrial and engineering applications.

Discrete meso-structural models are particularly appropriate to understand how the deformation mechanisms at the micro-structural level determine the macroscopic continuum response, as they allow to directly incorporate single paper fibres as individual constituents of the discrete fibrous network. In the literature, several publications deal with mechanical descriptions of paper based on stochastic analytical or computational network models (Cox, 1952; Ostoja-Starzewski, 1998; Stahl and Cramer, 1998; Bronkhorst, 2003; Ramasubramanian and Wang, 2007; Strömbro and Gudmundson, 2008; Strömbro and Gudmundson, 2008; Liu et al., 2010; Liu et al., 2011; Kulachenko and Uesaka, 2012). These approaches describe an individual paper fibre as a chain of trusses (e.g. in Cox (1952)) or beams (e.g. in Bronkhorst, 2003;

* Corresponding author at: Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands. Tel.: +31 40 247 5169.

E-mail address: e.bosco@tue.nl (E. Bosco).

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Ostoja-Starzewski and Stahl, 2000) that are connected to each other through inter-fibre bonds, which are generally identified with the nodes. Commonly, fibres are modeled with an axial stiffness only; in Schulgasser and Page (1988), the transverse properties are included as well. The existing network models are generally reliable in quantifying mechanical properties at the sheet level, either in the elastic (Ostoja-Starzewski and Stahl, 2000) or in the visco-elastic (Strömbro and Gudmundson, 2008; Strömbro and Gudmundson, 2008) or in the elasto-plastic (Bronkhorst, 2003; Ramasubramanian and Wang, 2007; Liu et al., 2011) range.

Effective hygro-expansive properties of paper can be obtained through a classical homogenization approach (Rosen and Hashin, 1970; Hashin, 1983), which provides hygro-expansive coefficients for a general anisotropic composite as a function of the hygro-elastic properties of the phases with an arbitrary geometry. Specifying the expression for a fibrous network is, however, not trivial. In Uesaka (1994), the hygro-expansive behavior of paper is interpreted through the analysis of the phenomena occurring at the mesoscopic scale. Both mechanical and hygro-expansive properties (in the longitudinal and transverse direction) of a single fibre contribute to the effective response of the material. In particular, the degree of macroscopic stress transferred within the network throughout the inter-fibre bonds governs the effective hygro-expansivity. An important role of hygro-mechanical interactions within fibre bonding zones is thus suggested. This approach can explain in a qualitative way a number of experimental results (Uesaka, 1994; Uesaka and Qi, 1994); however, a strategy to compute the hygro-expansive coefficients explicitly is not at hand. Also more generally, to the best of our knowledge, the literature lacks of models which are dedicated, based on the analysis of fibre level and network characteristics, to predict the resulting hygro-expansive behavior of paper.

In this contribution, a novel meso-structural model of paper is elaborated that bridges the hygro-mechanical properties at the fibre level to the effective response of the material. The fibrous network is simplified to a two dimensional periodic lattice structure, using a unit-cell with elements in four directions. The effect of the fibre orientation distribution, which is responsible for the paper's anisotropic behavior, is included in the geometrical characterization of the unit-cell. Free-standing fibre segments are considered as trusses. In the literature, a pin-jointed bond model is frequently adopted, see e.g. Bronkhorst (2003). However, this bond description is unrealistic, as the size of the bond (i.e. approximatively the fibre width) is of the same order as the inter-fibre spacing. Moreover, at the origin of the resulting hygro-expansive behavior of paper lies the coupling between the hygroscopic and mechanical properties of fibres in the bonding zones, which cannot be captured through pin-jointed bonds.

A distinctive aspect of this work is the fact that the inter-fibre bonds are modeled explicitly, and they are treated as laminated composite plates. The bonds incorporate both the longitudinal and transverse hygro-mechanical properties of the intersecting fibres, and thus contribute to the effective material response. Internal stresses in the bonds due to hygro-mechanical loads can be naturally represented. Elastic constitutive behavior has been considered for both fibre segments and bonds, restricting the present analysis to the macroscopic hygro-elastic behavior. However, in principle, different constitutive choices can be made for the meso-structural components in order to capture inelastic deformations and stress relaxation at the sheet level. The proposed lattice model is idealized, but for that reason extremely powerful. First, it can be solved analytically. Moreover, while allowing to extract the effective material properties in a simple manner, it offers additional insight in the elementary mechanisms connecting fibres up to the resulting behavior at the sheet level. All relevant features of the mesoscopic structure are explicitly taken into account: the geometry of fibres and bonds; the network structure through the fibre orientation distribution; and the anisotropic mechanical and hygroscopic properties of single fibres via their constitutive behaviors. Note finally that, even if the exact small scale constitutive and geometric parameters are not fully experimentally identified, the proposed model may help to understand qualitatively how sheet scale properties depend on network properties, and hence how to improve or tailor the macroscopic response by manipulating the network features.

This paper is organized as follows. In Section 2, the proposed meso-structural unit-cell model is defined together with the underlying assumptions on the network geometry and the fibre/bond constitutive behavior. The homogenization procedure used to extract the effective material properties is also detailed. An illustrative example is presented in Section 3, where the elastic and hygro-expansive properties calculated with the presented methodology are compared with experimental data extracted from the literature. Concluding remarks are given in Section 4.

Throughout the paper, the following notations for Cartesian tensors and tensor products are used: $a, \mathbf{a}, \mathbf{A}$, and ${}^n\mathbf{A}$ denote, respectively, a scalar, a vector, a second-order tensor, and an nth-order tensor. The following notation for vector and tensor operations is employed together with Einstein's summation convention: the dyadic product $\mathbf{a} \otimes \mathbf{b} = a_i b_j \mathbf{e}_i \otimes \mathbf{e}_j$, and the inner products $\mathbf{A} \cdot \mathbf{b} = A_{ij} b_j \mathbf{e}_i, \mathbf{A} \cdot \mathbf{B} = A_{ij} B_{jk} \mathbf{e}_i \otimes \mathbf{e}_k, \mathbf{A} : \mathbf{B} = A_{ij} B_{ji}$, with $\mathbf{e}_i$ $(i = x, y, z$ for the global reference system and $i = \ell, t, z$ for the local reference system) the unit vectors of a Cartesian vector basis. Voigt notation is used to represent tensors and tensor operations in a matrix form: a column and a matrix of scalars are indicated as $\underset{\sim}{a}$ and $\underline{A}$, respectively. The matrix multiplication is defined as $(\underline{A}\,\underset{\sim}{b})_i = A_{ij} b_j$, together with Einstein's summation convention.

2. Hygro-mechanical model

2.1. Target macroscopic model

The interactions at the meso-structural level between physical and geometrical properties of fibres play a fundamental role in determining the resulting material properties of paper. In order to assess the overall paper behavior, a macroscopic description must incorporate a detailed characterization of the fibres' mechanical response, dimensions, nature of inter-fibre bonds and the geometry of the network. From a macroscopic perspective, when a sheet of paper is exposed to a uniform change in the moisture content χ, the stress free hygro-expansive strain can be quantified as

$$\boldsymbol{\varepsilon}_h = \boldsymbol{\beta}\chi \tag{1}$$

where $\boldsymbol{\beta}$ is the tensor of effective hygro-expansive coefficients. If no external loads are applied, the average stress is zero, but internal stresses may arise in the fibre network. In addition, if macroscopic mechanical stresses are considered, in an elastic network, the total strain $\boldsymbol{\varepsilon}$ can be expressed as the sum of an elastic and a hygro-expansive part

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_h \tag{2}$$

and the following constitutive relation can be written

$$\boldsymbol{\sigma} = {}^4\mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\beta}\chi) \tag{3}$$

where ${}^4\mathbf{C}$ is the effective elastic stiffness tensor of the paper. The objective of this contribution is to predict $\boldsymbol{\beta}$ as well as ${}^4\mathbf{C}$, given the properties of the fibrous network.