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Research paper

Hygro-mechanical properties of paper fibrous networks through asymptotic homogenization and comparison with idealized models

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ABSTRACT

This paper presents a multi-scale approach to predict the effective hygro-mechanical behaviour of paper sheets based on the properties of the underlying fibrous network. Despite the vast amount of literature on paper hygro-expansion, the functional dependence of the effective material properties on the micro-structural features remains yet unclear. In this work, a micro-structural model of the paper fibrous network is first developed by random deposition of the fibres within a planar region according to an orientation probability density function. Asymptotic homogenization is used to determine its effective properties numerically. Alternatively, two much more idealized micro-structural models are considered, one based on a periodic lattice structure with a regular network of perpendicular fibres and one based on the Voigt average. Despite their simplicity, they reproduce representative micro-structural features, such as the orientation anisotropy and network level hygro-elastic properties. These alternative models can be solved analytically, providing closed-form expressions that explicitly reveal the influence of the individual micro-scale parameters on the effective hygro-mechanical response. The trend predicted by the random network model is captured reasonably well by the two idealized models. The resulting hygro-mechanical properties are finally compared with experimental data reported in the literature, revealing an adequate quantitative agreement.

1. Introduction

The dimensional stability of paper is a well known problem that affects several kinds of engineering applications, ranging from printing to packaging and storage operations. The response of paper to humidity variations is due to complex mechanisms originating at the level of the individual fibres (Niskanen, 1998). The moisture induced swelling of a single fibre is transferred to the entire network through the inter-fibre bonds, which play a crucial role in determining the macroscopic response. At this scale, paper may exhibit different types of in-plane or out-of plane deformations (Douezan et al., 2011). A key challenge is to understand how to bridge phenomena at the fibre and network level to the effective behaviour of paper, in order to formulate scale transition relations that allow to predict the effective response as a function of the properties of the underlying micro-structure.

The hygro-expansion of paper has been thoroughly investigated in the literature, mostly through experiments at the macroscopic scale, see e.g. Uesaka et al. (1992); Nanri and Uesaka (1993); Uesaka and Qi (1994); Niskanen et al. (1997); Torgnysdotter and Wagberg (2006); Larsson and Wagberg (2008); Erkkilä et al. (2015b). In these studies, the influence of several features of the fibrous network on the effective response has been analysed, for instance the inter-fibre bonds properties (Torgnysdotter and Wagberg, 2006; Larsson and Wagberg, 2008). Despite these valuable studies, an explicit, predictive relation between the micro-structural parameters, such as the hygroscopic and mechanical properties of the single fibre and the network structural characteristics, and macro-scale paper hygro-expansion has not yet been established.

A modelling approach can offer a substantial step forward in this direction. Classical homogenization provides the hygro-expansive coefficients of a general multi-phase material based on the hygro-mechanical properties of its constituting phases (Rosen and Hashin, 1970). The resulting relations are, however, formulated with respect to an arbitrary geometry, and their specification for a network of fibres is not trivial. In Uesaka (1994), a general formula for the hygro-expansive coefficients of paper is obtained as a function of the longitudinal and transverse hygro-expansions of the single fibres. These are related by weights incorporating the role

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of the hygro-mechanical interactions within the inter-fibre bonds of the network. Whereas the proposed formula can explain qualitatively the trend of some experimental results (Uesaka and Qi, 1994; Uesaka, 1994), it does not yet provide a quantitative estimate of the effective hygro-expansion properties for a specific network geometry.

The main goal of this work is to propose a multi-scale approach to calculate the effective hygro-mechanical properties of paper. This is done by developing a model of the underlying fibrous network and by studying its overall response through homogenization, by which the influence of the individual micro-structural parameters can be captured. In principle, different hypotheses can be made in formulating the model, which to some extent influence the results. In this paper, a dual strategy is followed. A detailed description of the network level *and* two highly idealized micro-structural models are developed and compared. As common assumptions, a two dimensional representation and perfectly bonded fibres are considered.

The first model is based on a periodic representative volume element (RVE) of the fibrous network, in which straight fibres are randomly positioned in the plane and follow a certain orientation distribution. This kind of description has analogies in the literature (Dodson, 1971; Sampson, 2009; Bronkhorst, 2003); the main originality here is the fact that the fibres are modelled as two dimensional domains, characterized by both longitudinal and transverse hygro-mechanical properties. The effective hygro-mechanical properties of the network are computed via asymptotic homogenization (Sanchez Palencia, 1980; Bakhvalov and Panasenko, 1989; Guedes and Kikuchi, 1990; Boutin, 1996) following the general procedure developed in Bosco et al. (2016). The method mainly consists in solving numerically a set of boundary value problems in relation to a given network geometry. This provides the displacement fluctuations at the network level due to mechanical and hygroscopic loads, which are needed to compute the effective elastic moduli and hygro-expansion coefficients. In the present manuscript, this methodology is specifically applied to paper. This includes the estimate of the effective material response using appropriate network properties, a comparison with experimental data and a study on the influence of the different material parameters within specific ranges typical for paper.

Alternatively, two idealized micro-structural models are proposed. The first one simplifies paper to a lattice structure, consisting of a unit-cell with elements in two orthogonal directions (Bosco et al., 2015c, 2015a). The effect of fibre orientation is included by defining weighted thicknesses for the fibres in the two directions, whose ratio is obtained by integration of the orientation distribution function. A key aspect of this approach is that, like the full network model, it distinguishes between the free-standing, unbonded fibre segments and the inter-fibre bonds. The model is solved analytically through homogenization, allowing to recover the hygro-mechanical response as an explicit function of the micro-structural properties. The second idealized description is based on the Voigt estimate, for which paper is considered a composite plate with an infinite number of layers oriented according to the probability density function.

A comparative study between the proposed methodologies is finally performed, to define their range of applicability and to identify their practical use for several industrially relevant applications.

This paper is organized as follows. In Section 2, the network model and the calculation of the effective hygro-mechanical material properties through asymptotic homogenization are proposed. The idealized descriptions of the paper fibrous network are detailed in Section 3. The comparison between the proposed approaches is made in Section 4, in terms of the resulting effective hygro-mechanical properties. Conclusions are finally given in Section 5.

2. Fibrous network model and asymptotic homogenization

The detailed fibrous network model and the asymptotic homogenization procedure to calculate the effective hygro-mechanical properties of paper have been developed in Reference Bosco et al., 2016. The main concepts are summarized here for the sake of clarity. Paper is approximated as a two dimensional material subjected to in-plane loads. A global reference system (x, y) is defined, which is aligned with respect to the material principal directions, the machine direction and the cross direction. The position vector reads $\mathbf{x} = x\mathbf{e}_x + y\mathbf{e}_y$, with $\mathbf{e}_i$, $(i = x, y)$ the unit vectors of a Cartesian vector basis.

2.1. Network geometry

The micro-structural fibrous network is described through the periodic repetition of a two dimensional unit-cell. Note that real paper micro-structures are not periodic. However, the unit-cell is assumed to be a representative volume element (RVE), which is sufficiently large to contain enough micro-structural information and to represent a real, stochastic paper network (Drugan and Willis, 1996). The RVE is assumed to be square, with edge L and area $Q : (0, L) \times (0, L)$. The geometry of each fibre is defined to be rectangular, with length l and width w. A rectangular cross section $w \times t$ is assumed, with t the thickness of the fibre. The fibres are positioned according to a uniform random point field, which determines the location of their geometrical centres $\mathbf{x}_c$ in the domain Q. Each fibre is characterized by an angle θ that follows a wrapped Cauchy orientation distribution probability density function (Cox, 1952):

$$f(\theta) = \frac{1}{\pi}\frac{1 - q^2}{1 + q^2 - 2q\cos(2\theta)} \tag{1}$$

where $-\pi/2 < \theta \leq \pi/2$ is the angle between the fibre axis and the $x-$direction (machine direction) and $0 \leq q < 1$ is a measure of the anisotropy of the network orientation. The portions of the fibres that fall outside the box $(0, L) \times (0, L)$ along a certain edge are trimmed and copied into the volume at the opposite edge. This ensures the periodicity of the RVE.

The number of fibres n_f of the network is characterized by the areal coverage $\bar{c}$,

$$\bar{c} = \frac{n_f wl}{Q} = \frac{b_p}{b_f} \tag{2}$$

defined as the ratio between the total area of the fibres and the area of the volume element. The last equality in (2) relates the coverage to the basis weight (i.e. the ratio between mass and area) of the fibres, b_f, and of the network, b_p; it will be used in the comparison with the idealized model of the network. Note that the coverage represents the average number of fibre layers characterizing the network and thus defines its average thickness to be $t\bar{c}$. During the network generation procedure, the fibres are deposited in the domain Q. Since the model is two dimensional, it is not possible to take into account the porosity of the system. The order of deposition is not considered, and all the fibres that overlap in a certain point of the domain are considered to be perfectly bonded to each other. Essentially, the thickness direction is collapsed into a plane, keeping track however, locally, of the number of fibres through the thickness and their orientations. The information on the average thickness provided by the coverage will be used to compute the local material properties, as discussed in Section 2.2.

Each fibre is treated as a two dimensional object. Generating a consistent finite element mesh for the complex network geometry may be cumbersome, especially in the bonds, in which two or more fibres with different orientations overlap. For this reason, a simplified procedure is adopted. A dense regular grid of square