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Transient transport of heat, mass, and momentum in paperboard including dynamic phase change of water

Henrik Askfelt*, Marcus Alexandersson, Matti Ristinmaa

Division of Solid Mechanics, Lund University, Box 118, 221 00 Lund, Sweden

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ABSTRACT

A theory to describe deforming moist paperboard in environments where both temperature and pressure change significantly during a short period of time is presented. Paperboard is viewed as an orthotropic triphasic porous medium consisting of fibers, bound water and moist air. Furthermore, the moist air is considered as a mixture of two miscible gases, namely dry air and water vapor. A two–scale hybrid mixture theory is adopted in a large strain setting and balances of mass, linear momentum, and energy are presented on the macroscale. Constitutive relations are derived on the macroscale through exploitation of the dissipation inequality. Mass exchange between bound water and water vapor is included as a dynamic process. Mass transportation processes include chemical potential driven diffusion and nonlinear seepage flow. The elasto–plastic stress–strain response of the fiber network is described by assuming a multiplicative split of the deformation gradient associated with the motion of the fiber network. The dynamics related to the mass exchange between bound water and water vapor is illustrated by changes of pressure, relative humidity, moisture ratio, and rate of evaporation during rapid heating of a moist paperboard.

1. Introduction

Paperboard is a porous medium consisting of three species: fibers, air and water. Fibers contain a cavity, called lumen, and have the approximate dimensions: length (1–5 mm), width (20–50 µm), fiber wall thickness (2–8 µm) (cf. Baggerud (2004)). Due to the paperboard making process, the board possesses a layered structure in the thickness direction and in the plane of the board a majority of the fibres tend to be aligned in one direction. The fiber alignment causes the paperboard to behave as an orthotropic material with three characteristic directions, Machine Direction (MD) and Cross machine Direction (CD), in the plane which constitutes the board, and the out–of–plane direction (ZD) which is a normal to this plane, cf. Fig. 1(a).

Water may be present in the inter–fiber pores, (0.5–10 µm), in the lumen, or in the intra–fiber pores, (5–10^4 Å), which are located in the fiber walls cf. Fig. 1(b). The properties of the liquid water differ depending on where the water is located. A majority of the water in the lumen and in the inter–fiber pores has the same properties as free water whereas water in the intra–fiber pores renders a reduced vapor pressure and an increased heat of adsorption due to interactions with fibers (cf. Baggerud (2004)). The moisture distribution in a paperboard has a direct influence on the properties of the paperboard

* Corresponding author.
E-mail address: henrik.askfelt@solid.lth.se (H. Askfelt).

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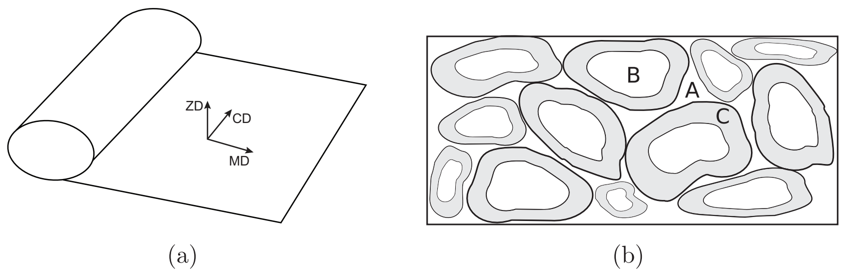

Fig. 1. (a) Illustration of the characteristic directions of paperboard and (b) illustration of the possible locations of water in paperboard (A) inter–fiber pores, (B) lumen, and (C) intra–fiber pores.

e.g. elastic modulus (Rigdahl, Andersson, Salmen, & Hollmark, 1984) and transport resistivities (Karlsson & Stenström, 2005; Linvill, 2015). The moisture distribution in a paperboard also has indirect consequences e.g. an affect on the pressure in the inter–fiber pores during temperature changes and the heat development during evaporation and condensation.

Considering the food packaging industry, which uses paperboard as their main packaging material, paperboard is exposed to many extreme environments where the moisture induced changes on the paper properties are known to cause problems. To be able to avoid these problems a better understanding is needed of how the moisture distribution in a board will change in different environments and also of how a known moisture distribution will affect the properties of a board, both directly and indirectly. In order to fulfil this need, a model capturing the coupling between moisture, temperature and deformations in paperboard is required.

Considering isothermal conditions and constant moisture content the stress–strain response of paperboard has been modelled in a large strain setting by e.g. Borgqvist, Wallin, Ristinmaa, and Tryding (2015); Harrysson and Ristinmaa (2008); Xia, Boyce, and Parks (2002). In these works, to capture the locally evolving mechanical anisotropy of paperboard local characteristic directions, i.e. structural tensors, are introduced following the framework outlined in Boehler (1987); Spencer (1984).

Models addressing a transient moisture–temperature interaction, without considering the stress–strain response, have been described in e.g. Alexandersson, Askfelt, and Ristinmaa (2016); Karlsson and Stenström (2005); Zapata, Fransen, Boonkkamp, and Saes (2013). In Zapata et al. (2013) paperboard is modelled as a two phase system. The evaporation is postulated to be a linear function of the sorption isotherm. The heat release from evaporation is addressed by including the isosteric heat in the balance of energy. In addition to the evaporation the moisture distribution is assumed to be affected by a Fickian inter–fiber vapor diffusion with a constant anisotropic diffusivity. In Karlsson and Stenström (2005) a triphasic model is presented where the moisture distribution is determined by a combined mass flux (including both vapor diffusion and gas bulk flow), liquid water diffusion and evaporation. The evaporation is postulated to follow Stefans equation. The isosteric heat is included in the energy balance and the constitutive parameters describing the kinetics of the transportation phenomena are considered to depend on the composition of the board. Alexandersson et al. (2016) adopt a hybrid mixture theory, HMT, and present a model where the constitutive functions are derived in a thermodynamically consistent manner. The moisture distribution is determined by a combined mass flux in the inter–fiber pore space and evaporation. Adopting a HMT framework Alexandersson et al. (2016) are able to derive general formats of the diffusion and the evaporation which are found to be driven by chemical potentials.

The aim of the presented article is to derive a model that is able to predict the response of deforming moist paperboard in environments where both temperature and pressure change significantly during a short period of time. The theory of mixtures is a class of methods that has been proven successful in describing this type of multi–physical problems. For the development of the theory of mixtures the reader is referred to Bowen (1976); Green and Naghdi (1967); Ingram and Eringen (1967); Kelly (1964); Müller (1968); Rajagopal and Tao (1995); Truesdell and Toupin (1960) and for extensive reviews of the historic development (Atkin & Crane, 1975; de Boer, 1992; 2000; de Boer & Ehlers, 1988; Bowen, 1976; Rajagopal & Tao, 1995).

A difficulty within the theory of mixtures is related to solving initial and boundary value problems. This stems from the fact that the mixture is viewed as a superposition of different continua and each continua is related to its own boundary/initial condition, whereas the considered problem usually only provides common boundary/initial conditions for the hole mixture. This aspect is considered in Rajagopal and Tao (1995); Rajagopal, Wineman, and Gandhi (1986) and will not be further elaborated in the present paper. To illustrate the capabilities of the developed theory, numerical examples that consider the dynamics related to the mass exchange between the bound water and the water vapor during a rapid heating of paperboard are provided.

2. Preliminaries

The present section provides a brief presentation of the kinematics concerning the theory of mixtures, for a more extensive overview (cf. Bowen (1976)). Adopting a mixture theoretical approach each point in a body is viewed as a super-