Construction and Building Materials 170 (2018) 716–724

Contents lists available at ScienceDirect

Construction and Building Materials

journal homepage: www.elsevier.com/locate/conbuildmat

The gripped-box model: A simple and robust formulation of sorption hysteresis for lignocellulosic materials

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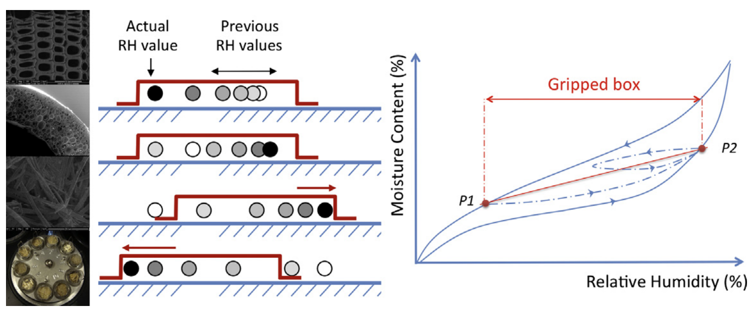
HIGHLIGHTS

- New formulation of sorption hysteresis for lignocellulosic materials.
- Easy implementation in existing computational softwares.
- The model ensures the closure of scanning loops after each wetting-drying cycle.
- An experimental RH sequence is proposed to identify the model parameters.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 2 January 2018
Received in revised form 16 February 2018
Accepted 18 February 2018

Keywords:
Water vapour sorption isotherms
Hysteresis
Modelling
No pumping effect
Wood
Wheat-straw
Flax-hemp
Cellulose

ABSTRACT

A new formulation is proposed for describing the moisture sorption hysteresis in lignocellulosic products. This model introduces the concept of gripped-box. This concept allows complex experimental pathways to be fitted with only two adjustable parameters, including the closure of scanning loops without any pumping effect. The product history is embedded in a unique internal variable, which defined the actual window of interest. The formulation proposed in the present work can be easily implemented in existing computational softwares. Based on comprehensive experiments, the model parameters were defined for five lignocellulosic materials largely used in the building construction.

1. Introduction

Due to the coupling between heat and mass transfer in building materials, the knowledge of the Equilibrium Moisture Content (EMC) as a function of ambient conditions is absolutely required in any modelling approach. Due to the importance of sorption hysteresis in lignocellulosic materials, this task is not easy as the value of EMC depends not only on the actual conditions, but also on the material history.

Sorption hysteresis is therefore an important aspect that needs to be taken into account in the study of material hygroscopicity. The reasons for sorption hysteresis depend of the porous media. In the presence of liquid water, whatever the pore size, the hysteresis can result from different effects, like the ink-bottle effect,

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https://doi.org/10.1016/j.conbuildmat.2018.02.116
0950-0618/© 2018 Published by Elsevier Ltd.

the variation in liquid–solid contact angle, the variations of size and spatial connectivity of pores [1]. For lignocellulosic materials in the lower range of EMC, the domain of bound water, the sorption history is likely to induce rearrangements of macromolecules, either by molecular mobility or at the ultrastructure level though the fields of strain/stress, for example between different cell wall layers. These macromolecular reorganizations play an important role in sorption hysteresis [2–6].

The sorption hysteresis is often neglected in the simulation of moisture transfer in building materials. However, omitting moisture hysteresis of sorption isotherm can lead to substantial errors in the houses design and on the computed indoor conditions namely with oscillating boundary conditions. For example it is well established that non-hysteresis modelling overestimates the moisture buffering capacity of the material [7], mainly because the actual slopes in the case of oscillation conditions are lower than those obtained at equilibrium, either for adsorption or desorption. Additionally, some works reported that the non-hysteresis modelling can lead to errors in the prediction of the moisture content up to 20%–30% (relative error) for wood sorption behavior [8]; in the estimation of the indoor comfort in terms of humidity and energy demand for heating [9] and in the moisture penetration depth within the material under drying-wetting cycles [10]. For concrete, omitting this effect is likely to underestimate the durability risks [11].

Different works [1,12] evaluated and discussed about the existing model for describing sorption hysteresis. They correctly pointed out that the classical independent domain model, which usually employs distribution diagrams to demonstrate the theory, is cumbersome to be implemented into numerical codes. Empirical models propose simpler formulations, which are easily implemented in computational models of heat and mass transfer in porous media. However, because they are developed without physical meanings for fitting the shapes of the experimental curves, it was observed for some materials like soil or cement that these models provide non-physical scanning loops (algorithm artefact), characterized by the so-called pumping error [1,13].

For lignocellulosic materials, these two modelling approaches have been proposed in literature. Some models, based on physical meanings, were applied and adapted to wood [8,14–17], or to hemp concrete [18]. Otherwise, different empirical models were used for fitting the shapes of the experimental curves of bio-based materials [12,19,20]. Frandsen et al. [12] proposed an interesting empirical model for wood easy to implement in computational softwares. In this model, the expression for the boundary curves can be chosen arbitrary. The hysteresis model required two shape parameters independent of the material and the temperature. The model is applied in [12] and [21] to fit experimental data available in literature for wood [22,23] and for concrete. But unusual mass changes in case of successive scanning loops were observed with this model for cement-based material [21]. These observations were explained by Zhang et al. [1] as an artefact of the model (also called pumping errors). For wood, Frandsen et al. [12] reported that the gradual moisture increase and stabilization during RH oscillation have also been observed in experiments by Chomcarn and Skaar [24]. Because the wood samples used in this latter work were some millimetres thick, this observation could be also explained by the moisture phase lag due to the characteristic time of diffusion. The validity of this empirical model was not tested with more complex sequences of RH in which the intermediate sorption curves are scanned in adsorption-desorption or vice versa. Otherwise, the Huang et al. model [25], used in [20] for hemp concrete, was designed to avoid such pumping errors of the hysteresis model and enforced the closure of scanning loops. Yet, it remains quite cumbersome when used in a computational model with frequent drying and wetting cycles, due to the need to rescale and reformulate each scanning curve when the RH-variations change in direction [1].

The main objective of this paper is to propose a new model for describing the sorption hysteresis of several lignocellulosic materials frequently used in building construction (wood, fibres from annual plants and cellulose). This model introduces the concept of gripped-box to propose a robust formulation easy to implement in computational software. In particular, it does not require the full history of relative humidity (RH) variations to be stored.

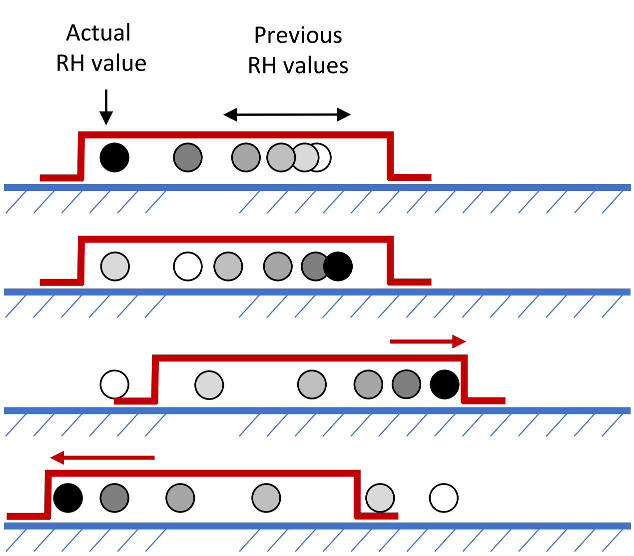

Fig. 1. The gripped-box concept: the box position does not change while the RH value remains inside the actual box position. On the contrary, the box moves as soon as the RH value attains one side of the box.

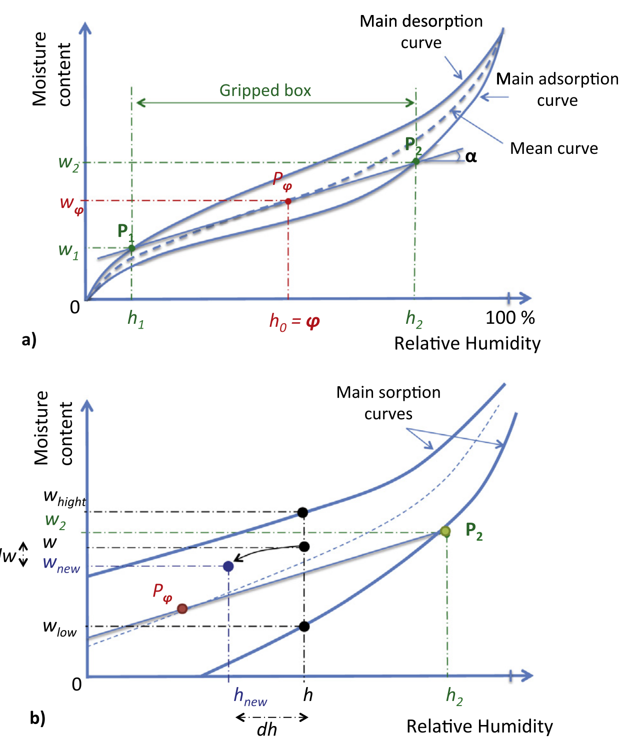

Fig. 2. Schematic drawing of the sorption curves with symbols used in the equations of the paper. Global view of the gripped box with the two target points P_1 and P_2 (a), and magnification with an example of one sorption step (b).