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A model of local kinetics of sorption to understand the water transport in bio-based materials

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Abstract. The classic models describing the hygric mass transfers inside porous materials seem unsuitable in the case of bio-based materials. They are based on the assumption of instantaneous local equilibrium between relative humidity and water content [1]. These two parameters evolve according to the diffusive fluxes following the sorption isotherms. This study shows that it leads to predict much shorter times of stabilization than those experimentally obtained. A new approach is presented here, it frees from the local instantaneous equilibrium introducing a local kinetics to describe the transformation of water from vapor state to liquid state and vice versa. The local kinetics of sorption is coupled with the well-known hysteresis phenomenon. It is adjusted from bibliographic data [2] giving mass evolution of three hemp concretes under adsorption / desorption conditions. 1D cylindrical simulations allows an excellent fitting on the experiments. Finally, a semi-empirical model is proposed, allowing to determine the kinetics parameters more easily. The effect of the local kinetics model on the hygrothermal transfers occurring through a bio-based wall is then studied.

Keywords: bio-based porous materials, hemp concrete, local kinetics, sorption, hygric transfer, modeling.

1 Introduction

Water sorption in porous media involves complex and coupled phenomena such as vapor / liquid water mass transport by Fickian diffusion and equilibrium isotherms of adsorption / desorption associated with hysteretic phenomena [3].

Classic simulation tools of hygrothermal transfers in building materials are based on the assumption that for a given local relative humidity (φ), the associated equilibrium local water content (w) is reached instantaneously. Here, various bio-based materials are studied: it is demonstrated that such an assumption leads to serious inconsistencies. Thus, a local kinetics of sorption may exist. It had already been established for bio-based materials [4, 5] as well as for traditional cement compounds [6].

The first part of this study is a summary of the hygric characterization performed on three selected hemp concretes [2] and on the bio-based materials developed during the ISOBIO project [7]. Then, the theoretical background necessary to model the

water sorption is presented. A new expression for the local kinetics of sorption is proposed and validated for the three studied hemp concretes in the following part. Then, a semi-empirical analytical model is proposed, allowing to estimate straightly the kinetic parameters. The final part studies a bio-based multilayered wall developed during the ISOBIO European project: simulations performed with a 1D Cartesian code based on the local kinetics model (TMCKIN) is compared against measurements carried out on a demonstrator (HIVE, Wroughton, UK).

2 Materials characterizations

2.1 Classic properties

The three studied hemp concretes are made of hemp shiv mixed with lime based mineral binders. Their properties had been characterized in [2]. The first one is a precast hemp concrete (PHC) also known as EASY-R™, the second one is a sprayed hemp concrete (SHC) and the third one is a molded hemp concrete (MHC).

The ISOBIO materials studied are: a BCB™ lime-hemp render (BCB), a CAVAC™ Rigid panel made of hemp shiv and an organic binder (CAV), a Biofib Trio flexible from CAVAC™ made of hemp wool (BIO), an OSB3, a Proclima™ INTELLO membrane (INT), a Lignicell CSB™ panel made of straw (CSB) and a CLAYTEC™ clay-hemp plaster (CLA). Their properties has been studied in [7].

Table 1 is a compilation of the classic properties of all these materials at dry state: the bulk densities ρ_0 , the open porosities ε_0 , the vapor diffusion resistance factors μ_0 , the thermal conductivities λ_0 and the specific heat capacities Cp_0 .

The Proclima INTELLO membrane is a hygrovariable material evolving very significantly as a function of the relative humidity RH following a logistic power law: $\mu = 1000/(7.33 \cdot 10^{-3} + 1.8 \cdot RH^{7.64})$. The evolution of the thermal conductivities as a function of the water content has been modeled by the self-consistent scheme [8].

Table 1. Materials classic properties

Mat.	ρ_0 ($\text{kg}\cdot\text{m}^{-3}$)	ε_0 (-)	μ_0 (-)	λ_0 ($\text{W}\cdot\text{m}^{-1}\text{K}^{-1}$)	Cp_0 ($\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$)
PHC	450	0.68	4	-	-
SHC	425	0.66	4	-	-
MHC	425	0.77	4	-	-
BCB	530	0.55	9	0.13	1006
CAV	197	0.43	9	0.07	2100
BIO	28	0.35	2.5	0.039	1800
OSB3	567	0.81	130	0.13	1600
INT	85	0.085	$1.37 \cdot 10^5$	2.74	2500
CSB	505	0.67	23	0.10	1700
CLA	1392	0.29	10	0.62	1040

2.2 Isotherms of sorption

The sorption isotherms were measured according to a discontinuous method: the time dependent water content W was determined at successive stages of increasing (and then decreasing) relative humidity at 23°C [2]. Note that for the ISOBIO materials, only the adsorption isotherm have been determined [7]. The measured equilibrium water content W_{eq} are fitted here by the Van Genuchten model (VG):

$$W_{eq}(RH) = W_{sat} \left[1 - (h \ln(RH))^\eta \right]^{1-1/\eta} \quad (1)$$

where W_{sat} is the maximum equilibrium local water content (*i.e.* $1000\varepsilon_0$) and h and η are adjustment coefficients. The adjustment coefficients are given in Table 2.

Table 2. VG model: adjustment coefficients

Mat.	h_{ads} (-)	η_{ads} (-)	h_{des} (-)	η_{des} (-)
PHC	166	2.05	258	1.65
SHC	378	1.77	500	1.46
MHC	185	1.98	75	1.66
BCB	8524	1.38	-	-
CAV	4830	1.435	-	-
BIO	198852	1.47	-	-
OSB3	25410	1.325	-	-
INT	2091	1.42	-	-
CSB	12966	1.334	-	-
CLA	12000	1.36	-	-

3 A model of local kinetics of sorption

3.1 Mass transport governing equations

Assuming that the rate of sorption R_s is very fast compared to the vapor diffusive flux (*i.e.* instantaneous equilibrium w / φ assumption), the mass transport can be described by the so-called Künzel single governing equation [1]:

$$\frac{\partial w}{\partial \varphi} \Big|_T \frac{\partial \varphi}{\partial t} - \nabla \cdot \left[\left(\frac{\delta_v}{\mu} P_{sat} + D_{p,l} \frac{\partial w}{\partial \varphi} \Big|_T \right) \nabla \varphi \right] = 0 \quad (2)$$

where $\partial w / \partial \varphi|_T$ is given by the isotherm of sorption.

Now, considering that the instantaneous equilibrium w / φ assumption is not justified, there are two mass balance equations to consider:

$$\begin{cases} \frac{\partial(\varphi P_{sat})}{\partial t} - \nabla \cdot \left[\frac{\delta_v}{\mu} \frac{RT}{M_w} \nabla(\varphi P_{sat}) \right] = - \frac{RT}{M_w} R_s \\ \frac{\partial w}{\partial t} - \nabla \cdot (D_{p,l} \nabla w) = R_s \end{cases} \quad (3,4)$$

Note that the coupling with a hysteretic model (*e.g.* [3]) can easily be done: the reversal points are obtained when the sign of R_s changes.

3.2 Sorption rate

A kinetics is usually expressed as a kinetic constant multiplied by a driving force. The simplest consistent expression that can be conceived for the sorption rate is the following:

$$R_s = k_0 (w_{eq}(\varphi) - w) \quad (5)$$

where k_0 is the local kinetic constant of sorption (adsorption or desorption) and w_{eq} is the equilibrium local water content given by the sorption isotherm at φ . [4] came to establish the same expression. However, the value of the kinetic constant k_0 has to be adjusted to quite different values as a function of the hygric conditions. Consequently, a more complex driving force has been established in our studies introducing a kinetic order of 2:

$$R_s = k_0 (w_{eq}(\varphi) - w)^2 \quad (6)$$

4 Validation of the local kinetics model

The model has been validated comparing the sorption curves measured by [2] performed on 5 cm diameter cylindrical samples of PHC, SHC and MHC to 1D cylindrical calculations. As evidenced by the results reported in Fig. 1a (adsorption) and 1b (desorption) for PHC, considering a value of k_0 of $2 \text{ day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$, the adjustments are globally very good. In adsorption conditions, the stabilizations of the water content occur from 5 days (at low RH) to several week at high RH . If the Künzel equation is considered instead, calculations lead to stabilizations in less than one day!

For SHC and MHC, the adjustments are also very good and lead to k_0 of $0.65 \text{ day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$ and $0.5 \text{ day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$ respectively.

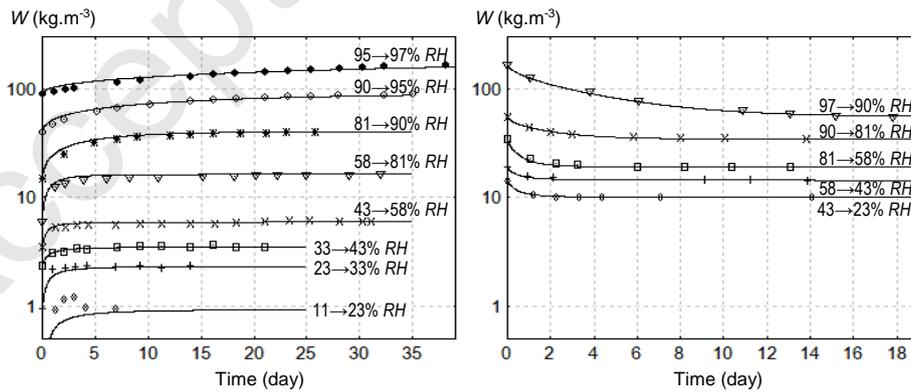


Fig. 1. Temporal evolution of the global water content W in a sample of PHC for (a) increasing / (b) decreasing RH steps - Experiments (points) and simulations (lines), $k_0 = 2 \text{ day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$.

5 A semi-empirical model for kinetic parameters identification

From [9] focusing on the hydration / dehydration of hydrated minerals, the global kinetics of water adsorption / desorption of a sample can be well described by:

$$W(t) = (W_i + W_f K_0 t) / (1 + K_0 t) \quad (7)$$

where K_0 (day^{-1}) is a global kinetic factor. Considering a kinetics order of 2, the following modified expression can be proposed:

$$W(t) = [W_i + W_f (W_f - W_i) K_0 t] / [1 + (W_f - W_i) K_0 t] \quad (8)$$

where K_0 is in $\text{day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$. Now, adjusting this model on the sorption curves, the agreement is good and the following values of K_0 are obtained: 1.75, 0.6 and $0.45 \text{ day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$ for PHC, SHC and MHC respectively. This is quite close to the values of the local kinetic constant k_0 deduced from the 1D cylindrical calculations.

6 Simulations of the HIVE demonstrator

An instrumented ISOBIO reference wall has been set up at the HIVE demonstrator (Wroughton, UK) by the University of Bath (UK). This reference wall consisted in (from outdoor to indoor): BCB, 25 mm; CAV, 50 mm; BIO, 145 mm; OSB3, 12 mm; INT, 0.25 mm; BIO, 45 mm; CSB, 40 mm and CLA, 15 mm. RH and T sensors were set up outdoor and indoor and at various positions inside the wall. The measurements have been performed in winter 2018 during 18 days, *i.e.* 434 hours

Some samples of these materials have been characterized [7], allowing, thanks to the semi-empirical model (eq. 8), to determine the following kinetic constant K_0 ($\text{day}^{-1}/(\text{kg}\cdot\text{m}^{-3})$): 0.0014 for BCB, 0.25 for CAV, 10 for BIO and 0.007 for CSB.

The simulations have been performed with two 1D Cartesian tools: TMC based on the Künzel equation and TMCKIN based on the local kinetics model. Fig. 2 shows the RH measurements and the results of the simulations at the interface BIO / OSB3: Contrary to TMC, TMCKIN predicts the good RH dynamics.

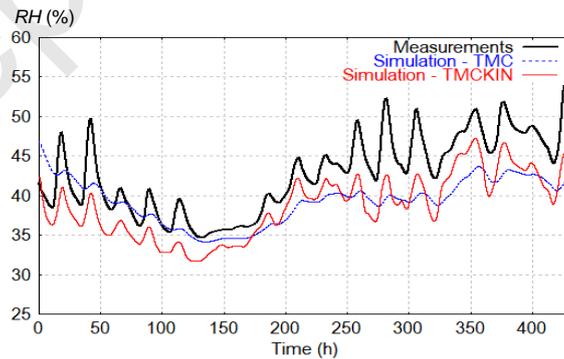


Fig. 2. Temporal evolution of RH at BIO / OSB3 interface – measurements and simulations (TMC and TMCKIN)

7 Conclusion

This study has allowed to understand, model and validate a new phenomenon: the local kinetics of sorption. An expression for the sorption rate has been established and validated.

Beside a homemade code named TMC based on the classic approach, a new 1D simulation tool named TMCKIN has been developed taking into account the local kinetics of sorption. Finally, the data acquired at the HIVE demonstrator inside the ISOBIO multilayered reference wall have been successfully simulated with TMCKIN. TMC underpredicts the dynamics of the RH variations (at the hour / day scale) while TMCKIN leads to results in good agreement with the measurements.

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