A LOCAL KINETICS OF SORPTION MODEL: THEORETICAL BACKGROUND AND APPLICATION TO THE SIMULATION OF AN ISOBIO DEMONSTRATOR

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Abstract

The classic models describing the hygric mass transfers inside building materials seem unsuitable in the case of bio-based materials. They are based on the assumption of an instantaneous local equilibrium between relative humidity and water content evolving according to the diffusive fluxes and the sorption isotherms and predict much shorter times of stabilization than those obtained experimentally. 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 absorbed liquid state and vice versa.

In the framework of the European ISOBIO project, a multilayered wall mainly made of bio-based materials has been developed. The different layers have been characterized in terms of sorption, vapor permeabilities and thermal conductivities. The sorption measurements performed on representative samples have allowed to determine the local kinetics constants. Then, the hygrothermal behavior of the test wall has been studied thanks to an instrumented demonstrator (HIVE demonstrator, Wroughton, UK). The recorded measurements are compared to simulations based on the instantaneous local equilibrium model (TMC code) and on the local kinetics of sorption model (TMCKIN code). It appears that TMC very significantly underestimates the dynamics of the local relative humidities variations whereas TMCKIN succeed in predicting this dynamics and leads to results close to measurements.

Keywords:

Bio-based materials; local kinetics; sorption; mass transfer; hygric transfer; modeling

1 INTRODUCTION

The aim of the European ISOBIO project was to develop multilayered wall solutions made of bio-based materials featuring very low carbon footprints and high insulating properties. The study presented here has been done in this framework. One of the key points of this project was to be able to perform proper simulations of the hygrothermal transfers occurring inside the ISOBIO reference wall.

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 also called "water storage functions" associated with hysteretic phenomena. The diffusion coefficients can be determined in steady state exchange by permeability measurements (i.e. "wet cup method" [Kumaran 1998]). The equilibrium isotherms of water sorption can be determined by gravimetric methods [Iglesias 1982]. The hysteretic phenomena is rather well understood and can be described by hysteretic models [Carmeliet 2005], [Huang 2005]. But despite the knowledge and the reliability of these hygric models, it seems that inside some porous materials, and

particularly the bio-based materials, such models largely underestimate the time required for the water content to reach the equilibrium: it has been established for bio-based materials [Nyman 2006], [Frandsen 2007], [Eitelberger 2011], [Alexandersson 2016] but also for more traditional material such as cement compounds [Johannesson 2010], [Zeng 2015]. These considerations take on their full meaning in the cases of hygric transfers with permanent fluctuations such as the hygric transfers occurring in materials of building envelops, in soils or in food materials.

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. In our previous studies [Reuge 2018], [Reuge 2019], three hemp-lime concretes were studied and it was demonstrated that such an assumption led to serious inconsistencies. Thus, as reported in the aforementioned literature, our previous studies have established that a local kinetics of sorption may exist (from water vapor to liquid water and inversely) which is slow compared to the diffusive fluxes. Obviously, this invalidate the classic assumption.

The first part of this study deals with the hygric and thermal characterizations performed on samples of ISOBIO materials. Then, the theoretical background necessary to model the water sorption is presented. Studies based on the simulations of hygric transfers during adsorption tests in samples of ISOBIO materials invalidates the calculations performed with traditional models using the assumption of instantaneous φ / w equilibrium. Then, a new and adequate expression for the local kinetics of sorption is proposed: the associated parameters are a kinetic constant and a driving force. The new mass transfer model is validated for the studied ISOBIO materials against experiments of global kinetics of adsorption. Moreover, a semi-empirical analytical model is proposed, allowing to estimate straightly the kinetic parameters. The last part of this study compare the results of the simulations based on the classic model and the local kinetic model to the measurements performed inside the ISOBIO reference wall at the HIVE demonstrator (Wroughton, UK) over a wide range of hygric and thermal operating conditions.

2 ISOBIO MATERIALS PROPERTIES

2.1 Experimental characterizations

The experimental characterizations of the ISOBIO materials hygrothermal properties are the subject of a second paper for this conference [Collet 2019]. Therefore, the experimental methods of measurements will not be described here but only the values of the properties necessary to perform the simulations.

The reference ISOBIO wall is composed of: 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 panel, a Proclima™ INTELLO membrane (INT), a Lignicell CSB™ panel made of compressed straw (CSB) and a CLAYTEC™ clay-hemp plaster (CLA). Note that this wall is supported by a timber frame which will not be considered in the 1D simulations.

Tab. 1 is a compilation of the following properties: the bulk densities at dry state ρ_0, the maximum water contents W_{sat}, the vapor diffusion resistance factors at dry state μ_0, the thermal conductivities at dry state λ_0 and the specific heat capacities at dry state Cp_0. Note that while most of these properties have been determined by [Collet 2019], a few others have been determined by other ISOBIO partners or obtained from trustable technical sheets.

	ρ_0	W_{sat}	μ_0	λ_0	Cp_0
	(kg/m^3)	(kg/ m^3)	(-)	(W/m.K)	(J/kg.K)
BCB	530	546	9	0.13	1006
CAV	197	427	9	0.07	2100
BIO	28	348	2.5	0.039	1800
OSB3	567	814	130	0.13	1600
INT	85	85	1.364 .10^5	2.74	2500
CSB	505	667	23	0.10	1700
CLA	1392	294	10	0.62	1040

Tab. 1: ISOBIO materials properties

The evolution of these properties with the water content will be investigated in the next section.

The adsorption behavior of representative samples of the ISOBIO materials have been studied by [Collet 2019] determining their water content W temporal evolutions until quasi stabilization (or in other words, their global kinetics of adsorption) after several instantaneous increments of ambient relative humidity RH at a temperature T of 23°C. For the CAVAC Rigid samples, the results of the measurements are presented in Fig. 1 for the following steps: 0→30%RH, 30→50%RH and 50→65%RH. The sample mass monitoring (allowing to determine W) has been continuous for the 0→30%RH and 50→65%RH steps (sample 1) and discontinuous for the 30→50%RH step (sample 2). The final stabilized W are actually the equilibrium water contents W_{eq} at the corresponding RH, allowing to determine the adsorption isotherm of the material. For the CAVAC Rigid material, the measurements of W_{eq} as a function of RH are presented in Fig. 2.

2.2 Models of properties

From the measurements of W_{eq} as a function of RH, the Van Genuchten model VG [Van Genuchten 1980] has been used to determine the adsorption isotherms. The VG model is claimed valid even at high RH (>90%). It is expressed as follow:

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

where and h and η are adjustment coefficients.

This VG model has been adjusted on the experimental data for every ISOBIO material. The values of the adjustment coefficients are given in Tab. 2 and the Fig. 2 shows the adjustment for the CAVAC Rigid material. Note that the adjustments has been performed to obtain the best possible correlations in the range of 40%-100%RH.

	h (-)	η (-)	λ_s
BCB	8524	1.38	0.312
CAV	4830	1.435	0.115
BIO	198852	1.473	0.048
OSB3	25410	1.325	0.809
INT	2091	1.42	2.73
CSB	12966	1.334	0.317
CLA	12000	1.36	0.995

Tab. 2: Adjustment coefficients – VG model and self-consistent scheme

The evolution of the vapor diffusion resistance factors μ as a function of the local water content w has been ignored except for the Proclima INTELLO membrane because it is a hygrovariable material evolving very significantly as a function of w. The data provided by Proclima have been fitted by a logistic power as shown in Fig. 3. Because of its great value, numerical tests revealed that this parameter is by far the most sensitive compared to the parameters μ of the other ISOBIO materials and then must be carefully modeled.

Finally, the evolution of the thermal conductivities as a function of the water content has been modeled by the self-consistent scheme [Collet 2014], which takes the following expression:
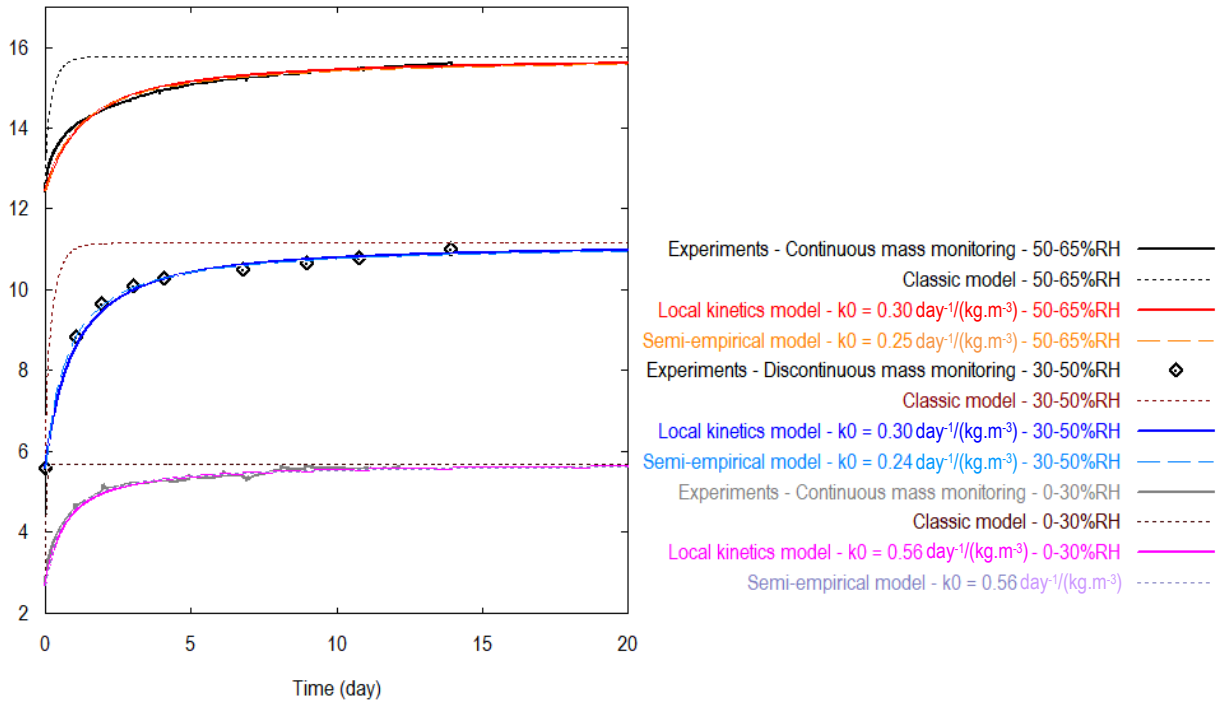
Water Content W (kg.m^{-3})

Fig. 1: Global kinetics of sorption of a CAVAC Rigid sample for three steps, 0→30%RH, 30→50%RH and 50→65%RH, T = 23°C – Measurements and simulations

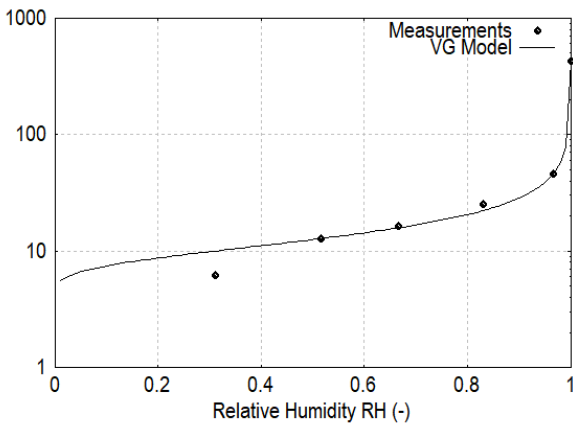Water Content W (kg.m^{-3})

Fig. 2: Adsorption isotherm of the CAVAC Rigid material – measurements and adjustment by the VG model

Fig. 3: Vapor diffusion resistance factors µ of the Proclima INTELLO membrane as a function of RH – Measurements and adjustment by a logistic power law – a = 7.3310^{-6}, b = 1.8.10^{-3} and c = 7.644

$$\lambda(W) = \lambda_s \left\{ 1 + \varepsilon_0 \left[\frac{1-\varepsilon_0}{3} + \left(3 + \frac{W}{1000\varepsilon_0} \left(\frac{0.025}{0.6} - 1 \right) \right) \right. \right.$$

$$\left. \left. \cdot \left(3 \left(\frac{0.025}{\lambda_s} - 1 \right) - \frac{W}{1000\varepsilon_0} \left(\frac{0.025}{0.6} - 1 \right) \left(2 \frac{0.6}{\lambda_s + 1} \right) \right)^{-1} \right]^{-1} \right\} \quad (2)$$

where ε_0 is the material open porosity. The coefficient λ_s (which can be seen as the thermal conductivity of the material skeleton) is adjusted such as $\lambda(W=0)$ equals λ_0. The values of λ_s are given in Tab. 2.
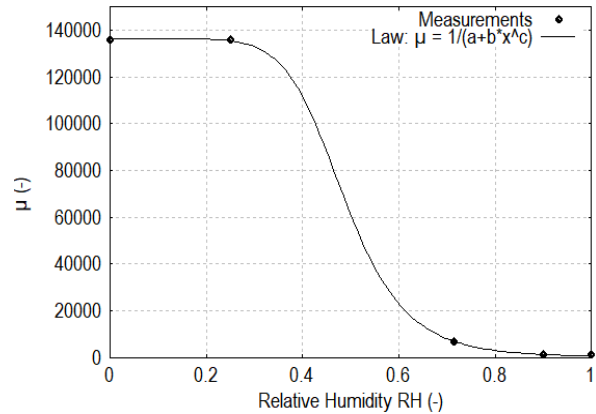
3 A MODEL OF LOCAL KINETICS OF SORPTION

3.1 Mass transport governing equations

In this section, (*i*) air transport is ignored. In the porous samples, water is present in gaseous form (water vapor) and in liquid form. Therefore, there are two mass balance equations to consider. Assuming that (*ii*) the convective transport is negligible, they take the following form:

$$\begin{cases} \dfrac{\partial \bar{\rho}_v}{\partial t} - \nabla \cdot \left(D_{p,v} \nabla \bar{\rho}_v \right) = -R_s \\[2mm] \dfrac{\partial \bar{\rho}_l}{\partial t} - \nabla \cdot \left(D_{p,l} \nabla \bar{\rho}_l \right) = R_s \end{cases} \qquad (3,4)$$

where $\bar{\rho}_v$ and $\bar{\rho}_l$ are the local water vapor and liquid water partial densities, $D_{p,v}$ and $D_{p,l}$ are the water vapor and liquid water diffusivities and R_s is the rate of sorption.

The local relative humidity can be expressed as follow:

$$\varphi = \frac{P_v}{P_{sat}} = \frac{\bar{\rho}_v RT}{M_w P_{sat}} \qquad (5)$$

and the local liquid water partial density $\bar{\rho}_l$ (*i.e.* the local water content) will be written by convention as *w*. Thus, eqs (3,4) can be rewritten as follow:

$$\begin{cases} \dfrac{\partial \left(\varphi P_{sat} \right)}{\partial t} - \nabla \cdot \left[\delta_{v,p} \dfrac{RT}{M_w} \nabla \left(\varphi P_{sat} \right) \right] = -\dfrac{RT}{M_w} R_s \\[3mm] \dfrac{\partial w}{\partial t} - \nabla \cdot \left(D_{p,l} \nabla w \right) = R_s \end{cases} \qquad (6,7)$$

where the porous media vapor permeability $\delta_{v,p} = \delta_v / \mu = D_v M_w / \mu RT$, the water vapor diffusion resistance factor being given by $\mu = \delta_v / \delta_{v,p} = D_v / D_{p,v}$.

It is commonly assumed that the rate of sorption R_s is very fast compared to the vapor diffusive flux. According to this assumption, the sorption process is limited by the diffusive fluxes and *w* moves along the isotherm of sorption $w_{eq} = w_{eq}(\varphi)_{|T}$. Assuming that (*iii*) the isotherm of sorption remains unchanged whatever the given temperature, we can write:

$$\begin{cases} \dfrac{\partial w}{\partial t} = \left. \dfrac{\partial w}{\partial \varphi} \right|_T \dfrac{\partial \varphi}{\partial t} \\[3mm] \nabla w = \left. \dfrac{\partial w}{\partial \varphi} \right|_T \nabla \varphi \end{cases} \qquad (8,9)$$

where $\partial w / \partial \varphi |_T$ is given by the isotherm of sorption. From eqs. (6, 7, 8, 9), the following single governing equation can be obtained:

$$\left. \frac{\partial w}{\partial \varphi} \right|_T \frac{\partial \varphi}{\partial t} - \nabla \cdot \left[\left(\delta_{v,p} P_{sat} + D_{p,l} \left. \frac{\partial w}{\partial \varphi} \right|_T \right) \nabla \varphi \right] = 0 \qquad (10)$$

Equation (10) is the so-called Künzel mass transfer equation [Künzel 1995].

Now, assuming that the rate of sorption R_s is not fast compared to the vapor diffusive flux, the two mass balance equations (6) and (7) must be considered. Then, the coupling with the hysteretic model of Huang et al. [Huang 2005] can easily be done: the reversal points (*i.e.* transitions between adsorption and desorption phases) are obtained when the sign of R_s changes.

3.2 Boundary conditions

At the wall or sample edge *edg$_i$*, the relative humidity is given by:

$$\varphi_{edg_i} = RH - \frac{\delta_{v,p}}{h_m} \cdot \nabla \varphi \big|_{edg_i} \qquad (11)$$

where h_m is the mass transfer coefficient and the water content is given by:

$$\nabla w \big|_{edg_i} = \left. \frac{\partial w}{\partial \varphi} \right|_T \nabla \varphi \big|_{edg_i} \qquad (12)$$

3.3 Sorption rate

Figure 1 shows the global kinetics of adsorption of a sample of the CAVAC Rigid ISOBIO material initially stabilized at given *RH* and submitted to higher ambient *RH*. From the measurements, the stabilization of the global water content *W* of the sample only occurs after 10 to 15 days.

According to the classic assumption of instantaneous local equilibrium between relative humidity and water content (according to the adsorption isotherms), 1D cylindrical calculations (*i.e.* with the Künzel equation) leads to a stabilization lower than 2 days (Fig. 1). This clearly shows that the classic assumption of instantaneous local equilibrium φ / w is not valid in these operating conditions.

Therefore, a relatively low kinetics of sorption may locally occur. It has already been noticed for different bio-based porous material such as wood [Frandsen 2007], [Eitelberger 2011] or paper [Alexandersson 2016] and various cellulosic materials [Nyman 2006]. It may be presumed that this finding is generalizable whatever the bio-based porous material. But not only this class of materials is concerned since some studies show that it is also the case for more "classic" compounds such as cement based porous materials [Johannesson 2010], [Zeng 2015]. It has also been evidenced for soils [Maraqa 2016].

A kinetics is usually expressed as a kinetic constant multiplied by a driving force. Some studies have proposed to express the driving force as a function of relative humidities with more or less success [Frandsen 2007], [Eitelberger 2011], [Alexandersson 2016], [Maraqa 2016]. The problem is that they consider an equilibrium relative humidity which is a priori not known for a local approach and/or they have to change the value of the kinetics constant according the operating conditions. Actually, it seems more natural to express the driving force as a function of the local water content and thus the simplest expression for the sorption rate is the following:

$$R_s = k_0 \left(w_{eq}(\varphi) - w \right) \qquad (13)$$

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 a local relative humidity φ.

[Nyman 2006] and [Johannesson 2010] came to establish the same expression. However, the value of the kinetic constant k_0 still have to be adjusted to quite different values as a function of the operating conditions: this is not really satisfactory, the local kinetic constant should only depend on the porous materials and not on the hygric conditions, at least as long as the hygric state is far from saturation.

Consequently, a more complex driving force has been established in our studies introducing a kinetic order *n*:

$$R_s = k_0 \left(w_{eq}(\varphi) - w \right)^n \qquad (14)$$

Thus, new calculations based on the local kinetics assumption have been performed adjusting the

parameters k_0 and n. As shown in Figure 1, experiments are properly reproduced using a constant value k_0 of 0.3 day^{-1}/(kg.m^{-3}) (for $RH > 30\%$) and a kinetic order n of 2. Note that the best adjustments are indeed obtained with these values.

Some previously obtained results [Reuge 2018], [Reuge 2019] dealing with three hemp-lime concretes led to the same conclusions, *i.e.* that a kinetic order n of 2 had to be considered and that the adjustments led to constant values of k_0 as long as RH was greater than 30%.

For bio-based materials, the origin of the local kinetics might be explained by the existence of bound water [Frandsen 2007], [Engelund 2012]. Once in liquid state, the liquid water molecules enter into the biological cells. Bound water molecules slowly diffuse in these cells and finally fill the porosities trapped between/around these cells and/or inside the matrix. Therefore, the apparent local kinetics might be ruled by the slowness of bound water diffusion. From [Engelund 2012], this kind of diffusion induces mechanical strains in the samples and its speed would actually be linked to the speed of relaxation of these mechanical strains. As aforementioned, the distributions of the porous networks may play a role too. Therefore, it seems that the origin of the local kinetics is extremely complex, this question would require further long and deep investigations and then the kinetic order of 2 might be physically justified.

3.4 Proposal of a semi-empirical kinetic model

Evaluation of the local kinetic parameters requires sufficient experimental data. Empirical models used to describe the kinetics of sorption may be helpful to limit the needed data. From [Brown 1980] and from the study of [Nguyen 2009] focusing on the hydration / dehydration of hydrated minerals, the global kinetics of water adsorption / desorption of a sample can be well described by the following empirical expression given in Table 3.2 of [Nguyen 2009]:

$$\frac{d\alpha}{dt} = K\left(1-\alpha\right)^p \alpha^q \qquad (15)$$

where W_i and W_f are the initial and final global water contents of the sample, K is a global kinetic factor and the exponent p and q are adjustable parameters. α represents the proportion of bound and/or trapped water. Assuming that q is a zero coefficient and p equals 2 (see [Reuge 2019] for justifications), eq. (11) leads to the following expression:

$$W\left(t\right) = \frac{W_i + W_f K_0 t}{1 + K_0 t} \qquad (16)$$

However, in this expression, K_0 (day^{-1}) is a first order kinetic constant. As shown in the previous section, the kinetic order n to consider should actually be of 2. Thus, the following modified expression, assuming a kinetic order n of 2, can now be proposed:

$$W\left(t\right) = \frac{W_i + W_f \left(W_f - W_i\right) K_0 t}{1 + \left(W_f - W_i\right) K_0 t} \qquad (17)$$

where K_0 is the adjustable global kinetic constant expressed in day^{-1}/(kg.m^{-3}).

Now, adjusting this model on the different RH steps reported in Figure 1, it leads to values of K_0 very close to the k_0 obtained from the local kinetic model and W temporal evolutions very close to the ones predicted the

local kinetic model and therefore to the measurements (see Figure 1). The results from [Reuge 2018] and [Reuge 2019] dealing with three hemp-lime concretes led to the same conclusions.

This is very interesting because it means that the kinetic constants can be well estimated from the adjustment of an analytical expression (eq. 17) instead from mass transfer simulations.

3.5 Kinetic constant of sorption

From the global kinetics of adsorption measured in the framework of the ISOBIO project and adjusting the semi-empirical model (eq. 17), it leads to the following values of the kinetics constant k_0 (day^{-1}/(kg.m^{-3})):0.0014 for the BCB render, 0.25 for the CAVAC Rigid panel, 10 for the Biofib Trio Flexible panel and 0.007 for the Lignicell CSB. Thus, there is a difference of four orders of magnitude between the lower and the higher values: each value of k_0 is intrinsic of each composite porous material and many factors can explain these differences, very probably the nature of the components, the distributions of the porous networks and the fractions of biomass.

4 SIMULATIONS OF THE HIVE DEMONSTRATOR

4.1 Experimental setup

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 the following several layers (from outdoor to indoor):

- BCB render, 25 mm thickness,
- CAVAC Rigid panel, 50 mm thickness,
- BIOFIB Trio Flexible panel, 145 mm thickness,
- OSB3, 12 mm thickness,
- Proclima INTELLO membrane, 0.25 mm thickness,
- BIOFIB Trio Flexible panel, 45 mm thickness,
- Lignicell CSB panel, 40 mm thickness,
- CLAYTEC plaster, 15 mm thickness.

RH and T sensors were set up outdoor and indoor and inside the wall: at the CAVAC Rigid / BIOFIB Trio interface (position pos1), at the BIOFIB Trio / OSB3 interface (pos2) and at the INTELLO membrane / BIOFIB Trio interface (pos3). These sensors were connected to a computer allowing real time monitoring.

4.2 Comparisons between the measurements and the TMC/TMCKIN simulations

The measurements have been performed by the University of Bath team in winter 2018 during 18 days, *i.e.* 434 hours, between Feb. 24th and Mar. 14th.

During this period, the measured outdoor and indoor RH are reported in Fig. 4 and the outdoor and indoor T in Fig. 5.

As shown by these Figures, the climate was humid and cold, with outdoor RH varying between 50% and 100% and outdoor T varying between -7°C and 12°C.

The simulations have been performed by our two 1D Cartesian modeling tools: TMC based on the classic mass transfer model (*i.e.* Künzel equation) [Oumeziane 2013], [Oumeziane 2014] and TMCKIN based on the local kinetics approach. Materials properties and models of properties described in section 2 have been used. As water storage functions, the isotherms of adsorptions have been considered (the isotherms of desorption have not be measured) and therefore no hysteretic phenomena have been considered.
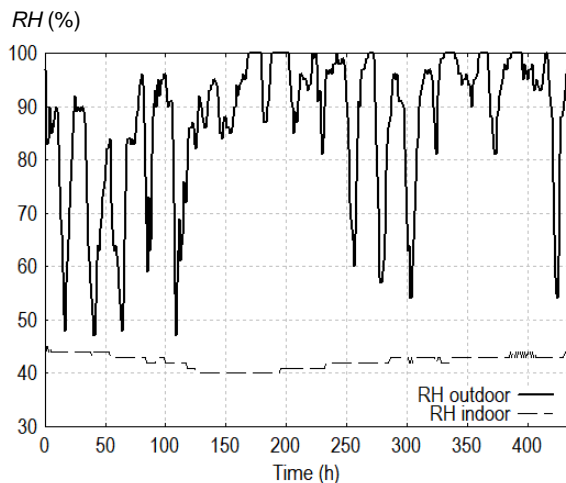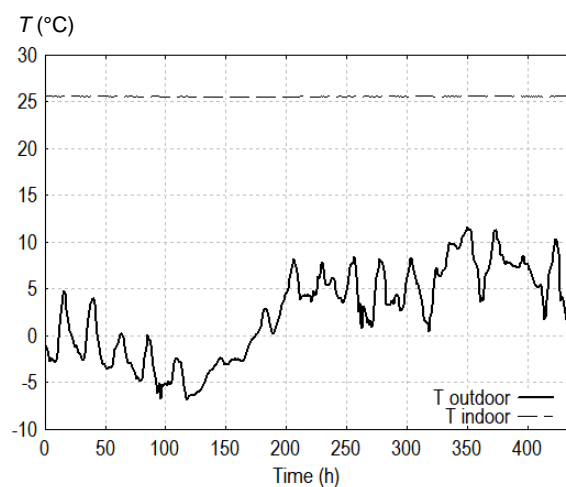
Fig. 4: Outdoor and indoor RH measurements

Fig. 6: Temporal evolution of RH at pos1 – measurements and simulations (TMC and TMCKIN)

Fig. 5: Outdoor and indoor T measurements

Fig. 7: Temporal evolution of RH at pos2 – measurements and simulations (TMC and TMCKIN)

For the TMCKIN simulation, the kinetics constants k_0 given in section 3.5 have been considered; the missing k_0 (CLAYTEC plaster and Proclima INTELLO membrane) have been considered equal to a standard value of 0.25 day^{-1}/(kg.m^{-3}). Standard outdoor and indoor heat and mass transfer coefficients have been applied at the wall surfaces. An initial RH of 80% has been considered into the wall with the associated W_{eq} for each layer. Actually, the true initial water contents in the layers were unknown, this fact leading to disagreements between measurements and simulations. In order to overcome this issue, first simulations were performed with TMC and TMCKIN with the aforementioned initial conditions over the entire period (434 h), the final local relative humidities and water contents inside the wall have been then used as initial conditions for second simulations performed over just a part of the period (250 h), the obtained final local relative humidities and water contents have been used again as initial conditions for third simulations performed over the entire period (434 h). The results presented here are those of these third simulations.

Fig. 6, 7 and 8 show the measured and calculated temporal evolution of RH at positions pos1, pos2 and pos3 respectively. Broadly, the calculated RH are relatively close to the measurements with maximum discrepancies of +/- 4%RH. But the TMCKIN results are remarkably better than the TMC results, the dynamics
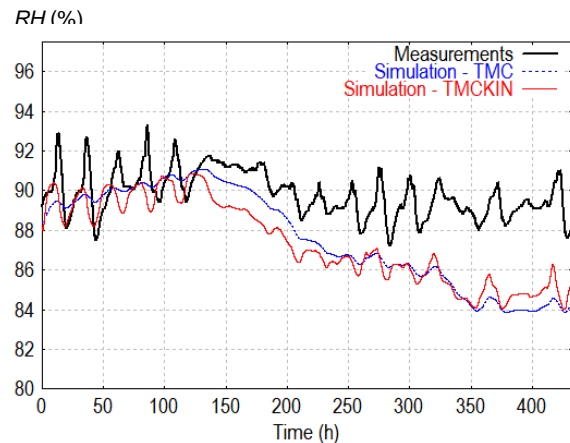

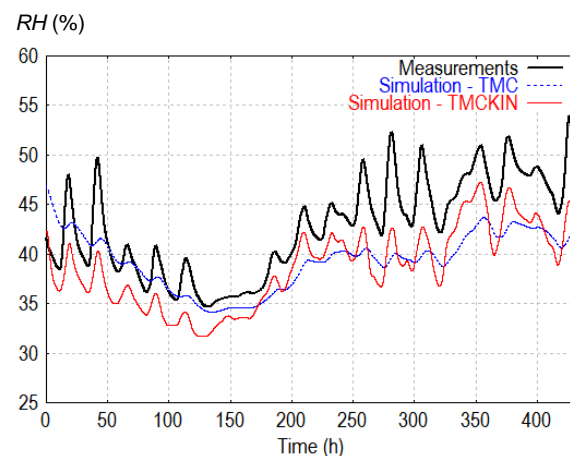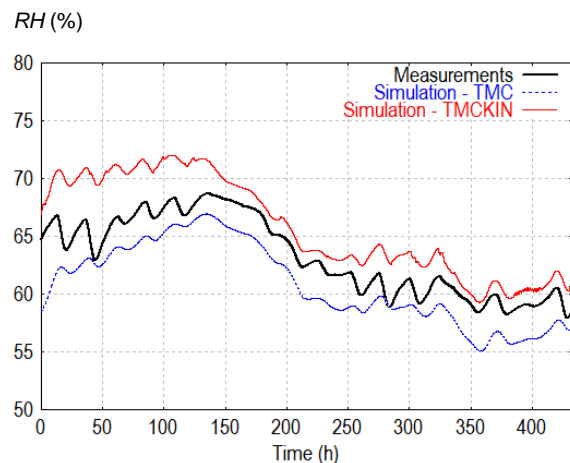Fig. 8: Temporal evolution of RH at pos3 – measurements and simulations (TMC and TMCKIN)

of the RH variations (at the hour / day scale) is close to the measurements whereas TMC don't catch this dynamics. This is obviously due to the effects of the local kinetics: slowing down adsorption and desorption phenomena, the large fluctuations of RH coming from outdoor are less softened. Therefore, these results can be considered as a good validation of the local kinetic model. The discrepancies between the measurements

and the TMCKIN simulation (+/- 4%*RH* at max.) might be due to not taking into account the real isotherms of desorption and the hysteretic phenomena.

The thermal results are not presented here because this study primarily focuses on the hygric transfers but overall, good agreements between measurements and simulations have been obtained.

5 SUMMARY

This study has allowed to understand, model and validate a new phenomenon: the local kinetics of sorption.

Thanks to measurements of global kinetics of sorption of ISOBIO bio-based materials and to simulations, it has been proved that the classic approach of Künzel based on the instantaneous local equilibrium between relative humidity and water content is not satisfactory in the case of bio-based materials. 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, thanks to the ISOBIO hygrothermal properties collected and modeled, 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.

6 ACKNOWLEDGMENTS

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