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Investigation on the use of hygrothermal modelling for paper collections

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Abstract. Dynamic simulation is increasingly adopted in the preventive conservation of cultural heritage as an advanced method to investigate strategies for mitigating the climate-induced degradation. The conservation of paper collections is strongly interrelated with the relative humidity of the air, as organic-hygroscopic materials act as buffers on relative humidity fluctuations while being vulnerable to moisture-induced damage. In the dynamic simulation of the microclimate within library and archival storage facilities, it is thus fundamental to include the hygrothermal interaction between the building and its hygroscopic content. The hygroscopic behaviour of paper collections can be modelled by hygrothermal tools such as those of the HAM-family (Heat, Air and Moisture), used to simulate simultaneous heat and mass transfers through porous envelope materials. This research aims at investigating the use of the HMWall model coupled with the software IDA ICE (Indoor Climate and Energy) to simulate of the 1-D heat and moisture transfer through a single wall made of paper. A literature survey was carried out to collect the available hygrothermal properties of modern and historical papers. Sensitivity analysis was used to identify the most relevant hygrothermal parameters in the simulation of moisture gradients across the paper wall. Moreover, the number of sub-layers in the paper wall model was found to significantly affect the internal distribution of moisture gradients. The use of the HMWall model was then tested in the simulation of the hygroscopic behaviour of a single paper wall in both steady-state and transient conditions. Finally, a simplified model able to preserve the accuracy of the results was proposed with the purpose of reducing the computation effort that a high-resolution model could involve if implemented in whole buildings. This study represents the first step towards the application of the HMWall model for the simulation of the indoor climate of library repositories.

1. Introduction

The conservation of library collections is strongly interrelated with the air relative humidity (RH) of the environment in which they are stored. In fact, organic hygroscopic materials are particularly vulnerable to moisture-induced damage due to chemical, biological and physical deterioration processes such as hydrolytic degradation, metabolic reactions and RH fluctuations affecting some properties of paper (e.g. pH and physical strength) [1]. Moreover, a reduction in the degree of polymerization and mechano-sorptive creep of paper can be accelerated under cycling humidity [2,3].

Whole-building dynamic simulation is being increasingly adopted in the preventive conservation of cultural heritage to study indoor environmental conditions and to investigate mitigation strategies of the climate-induced damages [4]. Hygroscopic materials effectively act as buffers on RH fluctuations [5−6] because they continuously exchange moisture with their surrounding environment. In modelling the environmental conditions within library and archival repositories, it is thus fundamental to include the hygrothermal interactions between the building and its hygroscopic content (i.e. the paper collections) [6−9]. Hence, a degradation scenario related to the microclimate conditions experienced by the library collections can be estimated using dose-response functions for paper [1].

The simulation of moisture transport through materials is complex as the properties of materials (particularly the historical ones) are frequently not fully known. The moisture buffering behaviour of paper collections is usually simplified by using the effective moisture capacity (EMC) approach, where the moisture buffering capacity of the indoor air is integrated with that of the books [6,9]. However, the hygrothermal response of cellulose-based objects can be more effectively modelled by means of tools commonly used for the simulation of the simultaneous heat and moisture transfer through porous envelope materials such as those of the HAM-family (Heat, Air and Moisture) [7,8,10,11]. In the simulation of moisture buffering effects, the HAM models are indicated as the most appropriate to account for moisture exchange in hygroscopic materials [12]. Steeman et al. [8] used a HAM model to simulate the hygrothermal conditions within a library repository and found the obtained results to be more accurate and reliable with respect to those obtained with the EMC approach. More recently, Kupczak et al. [7] have proposed a way to accurately model the water vapour diffusion in 3-D objects using 1-D moisture transport equations so that the buffering effects of paper collections can be precisely integrated. One must bear in mind that most of these studies focussed on the impact of the RH stabilization in terms of energy savings [7] and in the design of the air-conditioning systems [10] rather than on the implications on the conservation of paper collections. Furthermore, none of the above-mentioned studies investigated the uncertainties to be associated to the simulation outputs.

The HMWall model (hereafter called HMWall), based on Künzel equations [13] can be coupled with the modular software IDA ICE (Indoor Climate and Energy) to provide reliable dynamic hygrothermal simulations in historic buildings [4]. In Frasca et al. [14], the simulation performance of HMWall in IDA ICE was assessed through the comparison with the validated software WUFI Plus [15,16] and improved in its hygric part. To the authors' knowledge, HMWall has never been tested so far in modelling the hygrothermal conditions within library and archival repositories.

The hygrothermal properties of paper available in literature are measured following various procedures; moreover, as they depend on both the constituent materials and the manufacturing process, modern [6,7,9,20] and historical [19] papers can have rather different hygrothermal properties. Sensitivity Analysis (SA) can be used to determine which are the most influential parameters in the computation of the simulation results and to quantify their effect on the variability of the outputs. Since SA results are strongly related to the specific configuration to be tested, the analysis must be performed in relation with the modelling goals, carefully choosing the variability of the input parameters [17]. A recent work conducting a sensitivity analysis on the Künzel model found that thermal conductivity in a single layer wall of concrete can influence the water content distribution [18].

This paper aims at investigating for the first time the capability of HMWall coupled with IDA ICE 4.8 to simulate the dynamic moisture transport across a single wall made in paper at both steady-state and transient boundary conditions. A satisfactory performance of this coupled model will allow to move forward to the modelling of the whole-building hygrothermal behaviour of paper storage environments and to the implementation of methods for the preventive conservation of library and archival collections.

2. Materials and methods

The approach followed in this study includes five main steps:

- literature survey on the available hygrothermal properties of modern and historical paper;
- minimization of the discrepancy between the hygrothermal curves calculated by HMWall and those provided in literature;

- sensitivity analysis on the influence of the variability of the hygrothermal properties found in literature on the simulation outputs of a single paper wall;
- study of the effect of the number of sub-layers in the paper wall model on the computation of moisture gradients;
- investigation on the use of HMWall to simulate the hygroscopic behavior of a paper wall both in steady-state and in transient conditions.

2.1. Background information on HMWall

The HMWall model, whose underlying physical laws are thoroughly discussed in the PhD dissertation of Künzel [13], is based on the balance equations for heat and moisture transfers. In this 1-D fully coupled heat and mass model, the hygrothermal variables are strongly linked to each other since the thermal conductivity, which drives the heat transfer, is moisture-dependent and because the enthalpy flux is a function of both temperature and vapour diffusion flux.

In HMWall, the adsorption isotherms are calculated only as a function of relative humidity (φ), since the equilibrium water content (w) is assumed to be little sensitive to temperature changes and the hysteresis between adsorption and desorption is usually considered negligible. The moisture storage curve of the material is computed as follows:

$$w(\varphi) = w_f \cdot \frac{\varphi \cdot (b-1)}{b-\varphi} \qquad (1)$$

where w is the equilibrium water content (kg/m^3) corresponding to the relative humidity φ, w_f is the moisture content at free water saturation and b is an approximation factor calculated from the equilibrium water content at $\varphi = 0.8$ (w_{80}).

The diffusion of the material is expressed as a function of the dry diffusion resistance factor (μ). Capillary liquid water transport is described as a diffusion phenomenon in the material pore spaces regulated by the water absorption coefficient. The thermal conductivity of dry materials (λ_0) increases linearly with moisture content and is expressed as a function of the moisture-induced conductivity supplement (s), i.e. the fractional increase of λ_0 per percentage of moisture mass, which is mostly independent of the bulk density in the case of hygroscopic materials.

2.2. Hygrothermal properties of paper from literature

A literature survey was conducted to obtain an overview of the available experimental hygrothermal properties of common types of paper in library and archival repositories.

Table 1. Hygrothermal properties of modern* and historic** paper according to literature references.

References	ρ	C_p	λ_0	μ	w_f	w_{80}
	kg/m^3	J/(kg·K)	W/(m·K)	-	kg/m^3	kg/m^3
* [6,9]	690	750	0.06	87	165	95
* [7]	618	-	-	-	61	52
** [19]	-	-	-	-	105	76
* [20]	839	1150	0.09	-	-	-

Table 1 summarizes the values of bulk density (ρ), specific heat capacity of dry material (C_p) and dry thermal conductivity (λ_0) according to recent experimental works about paper. The value for water vapour diffusion resistance factor in dry conditions (μ) was obtained at RH=50% applying the formula in [6,9]; the values of w_{80} and w_f refer to the parameters of the HMWall moisture storage curve (Equation 1) fitted on literature data as will be described in the next paragraph. The hygrothermal properties of modern paper were measured on telephone-book paper [6,9], contemporary book paper [7] and offset uncoated paper [20], while the moisture coefficients in [19] are specific for historical cellulose-based paper. References [6,9] considered standard values for C_p and λ_0, whereas [7,19] did not provide any value for these parameters; therefore, reference [20] was introduced and used as a benchmark for the thermal properties of modern paper.

2.3. Modelling the hygroscopic behaviour of a paper wall with HMWall

The moisture storage curve of the various types of paper were first reconstructed according to the literature fitting equations and parameters. Then, the approximating parameters of the HMWall moisture storage curve in Equation 1 were chosen so that the discrepancy between the equilibrium water content values (w) in literature and those computed with HMWall was minimized at a benchmark value of ϕ=0.5 (Figure 1). The benchmark value was chosen as it encompasses the recommended conditions for the preservation of library collections, i.e. those targeting to avoid the risk of paper becoming brittle (at low ϕ) and the risk of mould growth (at high ϕ) [1].

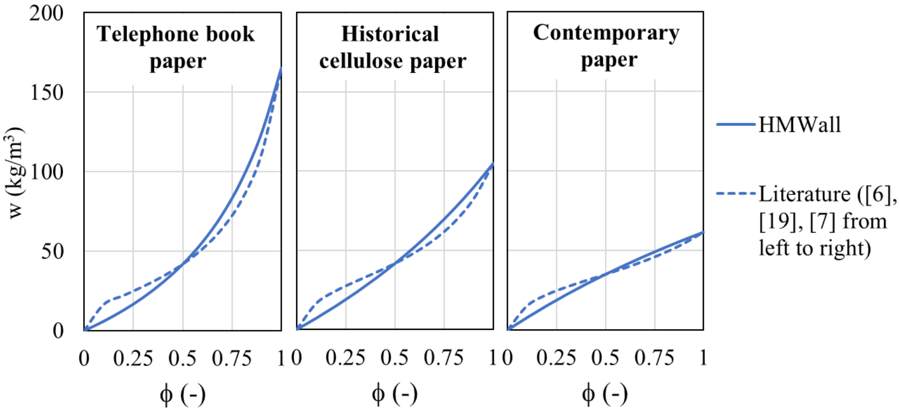

Figure 1. Moisture storage curves of paper from literature data (dashed lines) *versus* those computed by HMWall (solid lines). The discrepancy is minimized at ϕ = 0.5.

A preliminary sensitivity analysis (SA) was considered necessary to identify the most relevant hygrothermal parameters in the model influencing the moisture gradients across the paper wall (ΔRH), thus allowing to select among the various hygrothermal properties found in literature. For example, since the heat and moisture fluxes are balanced, the thermal properties driving the heat transfer could have an impact on the water content distribution in hygroscopic materials [18].

3. Results and discussion

The sensitivity analysis was conducted by using the Elementary Effects (EE) method based on the Morris random sampling method [17]. A HMWall single wall with area equal to 1 m^2, thickness 0.2 m and divided into N=63 sub-layers, was preconditioned at paper wall temperature T_{wall}=20°C and relative humidity RH_{wall}=50% and connected to identical boundary conditions of T=20°C and RH=70% (Figure 2). N was chosen in order to have a detailed model able to describe the heat and moisture transfer phenomena in paper, with thickness of each sub-layers equal to 3 mm.

The Morris random sampling considered 10 EE for each parameter and 4 discretized levels to span within the ranges of the selected hygrothermal parameters summarized in Table 1. Water liquid transport was assumed to be negligible for the scopes of this investigation and thus the vapour absorption coefficient was set to the minimum.

Table 2. Ranges of the selected hygrothermal properties of paper tested in the sensitivity analysis.

Sensitivity analysis inputs	Range
Density (ρ)	600−900 kg/m³
Specific heat capacity (C_p)	700−1200 J/(kg·K)
Dry thermal conductivity (λ_0)	0.05−0.10 W/(m·K)
Thermal conductivity supplement (s)	1.0–5.0
Free water saturation moisture content (w_f)	100−200 kg/m³
Equilibrium moisture content at RH = 80% (w_{80})	50−100 kg/m³
Dry vapour diffusion resistance factor (μ)	50−100

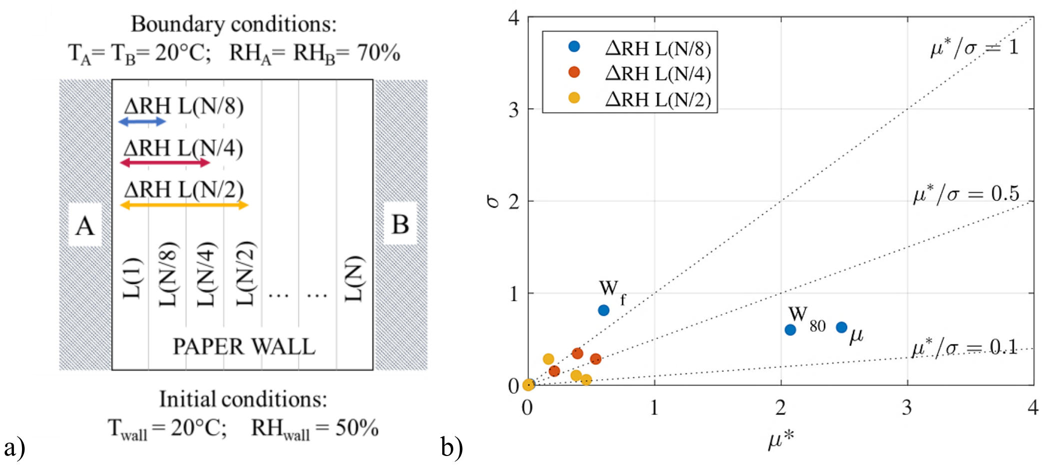

Figure 2. Scheme of the configuration of a paper wall model divided into N sub-layers (a); results of the sensitivity analysis (b) in terms of the mean (μ*) and the standard deviation (σ) of the Elementary Effects (EE) calculated on the RH gradients (ΔRH) after one month at the steady-state conditions described in a) with N=63.

The results of the sensitivity analysis showed that only the equilibrium moisture content at RH=80% (w_{80}) and the vapour diffusion resistance factor (μ) have a significant but low impact on the RH gradient (ΔRH) among the outermost sub-layers of a paper wall (ΔRH L(N/8) in Figure 2a); the remaining hygrothermal properties seem to have a negligible effect on the chosen output. In the light of the above considerations, for the simulation in HMWall it was reasonable to choose the set of parameters given in [6,9] because more complete (Table 3).

Table 3. Hygrothermal properties of paper used in this study.

Hygrothermal properties of paper	Value
Density (ρ)	690 kg/m^3
Specific heat capacity (C_p)	750 J/(kg·K)
Dry thermal conductivity (λ_0)	0.06 W/(m·K)
Thermal conductivity supplement (s)	1.0
Free water saturation moisture content (w_f)	165 kg/m^3
Equilibrium moisture content at RH = 80% (w_{80})	95 kg/m^3
Dry vapour diffusion resistance factor (μ)	87
Liquid water absorption coefficient (A)	1.0×10^{-11} kg/(m^2·s$^{0.5}$)

The influence of the number of N sub-layers in a single paper wall preconditioned to T_{wall}=20°C and RH_{wall}=50% was explored after one month of prolonged exposure to boundary steady-state conditions of T=20°C and RH=70%. Figure 3 shows a comparison among the RH values obtained at the same wall sub-layers as a function of the number N of equally-spaced sub-layers. The thicknesses (t) associated to N=63,31,15,7 sub-layers are t=3,6,13,29 mm, respectively. The high-resolution paper wall (N=63, t=3 mm) was chosen as reference. The results highlighted that a significant underestimation can be introduced in the computation of the internal RH gradients if the simulation is run using a paper wall model with a too low number of sub-layers because of the averaging over a too large sub-layer thickness.

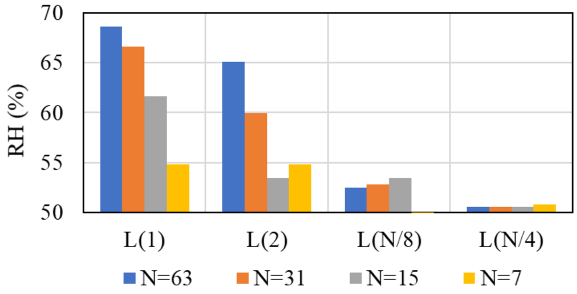

Figure 3. Relative humidity values (RH) after one month at the conditions described in Figure 2a obtained in correspondence with the same wall node as a function of the number of sub-layers (N). The sub-layer thickness (t) associated to N=63,31,15,7 sub-layers is t=3,6,13,29 mm.

In Figure 4 are shown the RH values obtained across the high-resolution paper wall as a function of the duration of boundary adiabatic conditions (T=20°C) and of the steady-state RH gradient from the preconditioning value (RH=50%) to RH=70%. The RH distribution within the paper wall evolves slowly, showing a significant variation starting from one week of prolonged exposure and reaching the full equilibrium between the bulk and the surfaces only after several years.

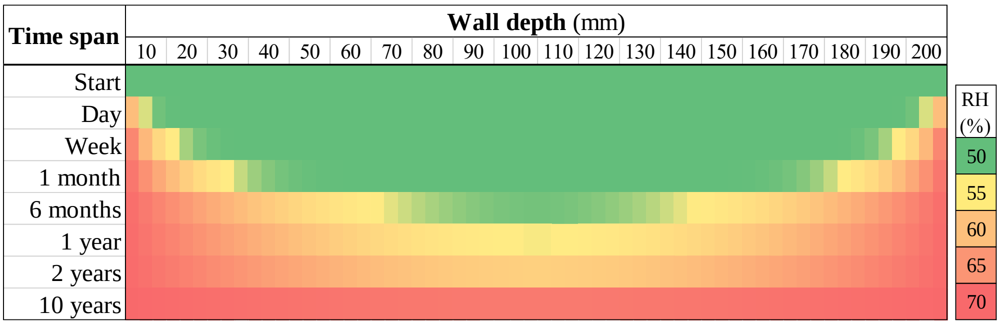

Figure 4. Relative humidity values (RH) within the paper wall as a function of the duration of the steady-state boundary conditions described in Figure 2a.

The influence of transient boundary conditions was also investigated for the case of a single paper wall having 63 equally-spaced sub-layers and being initially conditioned to T_{wall}=20°C and RH_{wall}=50%. The configuration was tested at boundary constant temperature T=20°C and RH conditions periodically ranging from 30% to 70% at weekly, monthly and seasonal frequency. The results in Figure 5 emphasised that the first 5 sub-layers (corresponding to the first 15 mm from the wall surface) are the most responsive to the external transient forcing. For the seasonal cycle, only RH variations above the threshold of +10% and below the threshold of −10% from the preconditioning value of RH_{wall} are shown.

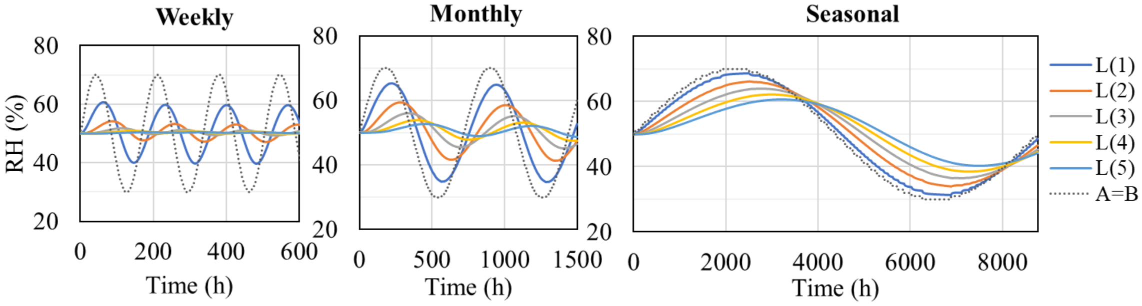

Figure 5. Relative humidity values across a paper wall divided into N=63 equally-spaced sub-layers at constant T=20°C and boundary RH conditions periodically ranging from 30% to 70% at weekly, monthly and seasonal frequency (grey dotted lines).

Even if high-resolution models can provide more accurate results, they may increase too much the computation effort needed to run the simulation when included in whole-buildings. For this reason, a simplified paper wall model was proposed as schematized in Figure 6. The simplified paper wall model has a reduced number of unequally-spaced sub-layers. The first 5 sub-layers located under the surfaces A and B (i.e. L(A) and L(B)) are assigned the same thickness as that of the high-resolution reference sub-layers (3 mm). The impact of the inner layers' thickness on the outputs was tested and found to be negligible. Hence, the minimum number of 3 was chosen for the inner sub-layers.

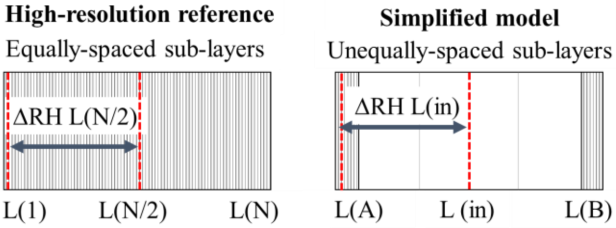

Figure 6 Scheme of the high-resolution paper wall divided into equally-spaced sub-layers (left) and the simplified paper wall divided into a reduced number of unequally-spaced sub-layers (right).

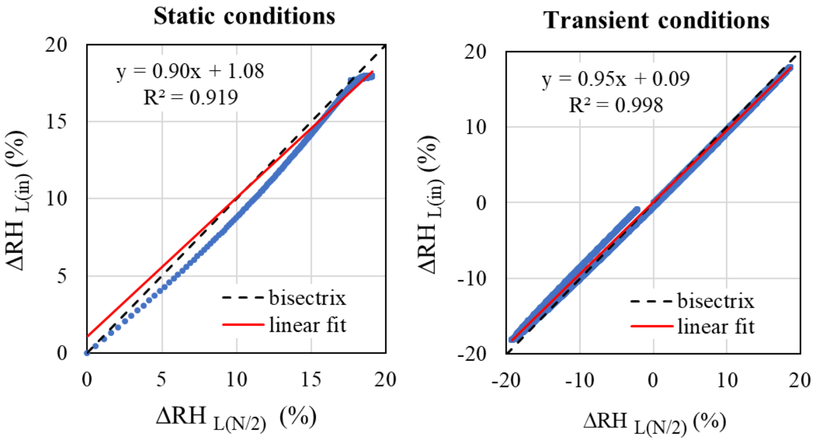

Figure 7. Scatterplot of hourly relative humidity gradients between the surface and the bulk of a paper wall over a year at the steady-state conditions described in Figure 2a (left) and at the transient seasonal conditions described in Figure 5c (right). $\Delta RH_{L(N/2)}$ and $\Delta RH_{L(in)}$ refer respectively to the RH gradients of a high-resolution model with N=63 equally-spaced sub-layers and of a simplified model with N=13 unequally-spaced sub-layers (see Figure 6).

The simplified model was tested in comparison with the high-resolution reference in terms of the RH gradient between the surface and the centre of the paper wall. As explained in Figure 6, the gradient $\Delta RH_{L(N/2)}$ of the high-resolution paper wall was calculated as the difference between the RH of the exterior sub-layer L(1) and that of the central sub-layer L(N/2), while the gradient $\Delta RH_{L(in)}$ of the simplified paper wall model is the difference between the RH of the exterior sub-layer L(A) and that of the central sub-layer L(in). Figure 7 shows a scatterplot of the $\Delta RH_{L(N/2)}$ *versus* $\Delta RH_{L(in)}$ calculated on a hourly basis over a year at both steady-state and transient seasonal conditions. The linear curve fitted on the results points out that the gradients in the simplified paper wall accurately reproduce those obtained with the high-resolution reference, therefore the proposed model can be used as a reliable alternative to reduce the simulation effort without losing accuracy in the results.

4. Conclusions

This paper aimed at investigating for the first time the capability of the HMWall model coupled with IDA ICE 4.8 in the simulation of the 1-D moisture transport across a single paper wall at both steady-state and transient boundary conditions. An initial literature survey has provided the available hygrothermal properties measured in paper. The results of a sensitivity analysis on a single paper wall exposed to an increase of the boundary relative humidity showed that paper thermal properties have a negligible impact on the water content distribution, whereas the equilibrium moisture content and the vapor diffusion resistance factor resulted to be the most influencing parameters on the tested output. The number of sub-layers used in the model significantly affect the relative humidity outputs at various depths within the paper wall. Nevertheless, since high-resolution models involve substantial computation effort when integrated in whole buildings, a simplified model able to keep the accuracy in the results was proposed. This preliminary investigation will be useful for an “informed use” of HMWall in the hygrothermal simulation of the indoor climate of library and archival repositories.

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