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Modelling the Similarity and the Potential of VOC and Moisture Buffering Capacities of Hemp Concrete on Indoor Air Quality and Relative Humidity

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ABSTRACT

The means for keeping the indoor relative humidity (RH) and pollutant concentration below a threshold level of interests are necessary and essential to improving building performance in terms of indoor air quality (IAQ), energy performance and durability of building materials. In this paper, the similarity between the moisture and VOC (Volatile Organic Compounds) transport models is applied to study the effect of toluene (a typical VOC) and moisture buffering capacities of a hemp concrete wall on indoor toluene concentration and RH. A numerical model which can be used to simulate VOC emissions from materials under dynamic conditions is presented. The model is implemented in the environment SPARK (Simulation Problem Analysis and Research Kernel) which is suited to complex problems using finite difference technique with an implicit scheme. The pollutant transport and storage properties obtained from hygrique properties of hemp concrete based on the assumption of the similarity between toluene and moisture transport has been presented. At the room level, the results obtained show that taking into account the sorption capacity toward moisture and toluene has a significant effect on hygric comfort and IAQ because hemp concrete contributes to dampen indoor RH and VOC variations. The numerical model presented is very useful for the building design optimization and can be used for a fast estimation of indoor pollution and hygrothermal conditions in a room.
Keywords: *Hemp concrete, moisture, toluene, VOC, buffering capacity, Indoor Air Quality, numerical model*

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INTRODUCTION

For evaluating the indoor air quality and thermal comfort, concentrations of pollutants such as the volatile organic compounds (VOC), indoor temperature and relative humidity in building are the most important factors. It has been shown that one of passive ways to keep the variation in RH between threshold levels in order to save energy and improve the indoor quality is the use of the moisture buffering capacity of materials (including the building envelope as well as interior objects) (Olalekan and Simonson 2006; Woloszyn et al 2009, Tran Le et al 2010). Regarding volatile organic compound (VOC), some studies showed that there is a similarity between moisture and VOC diffusion through porous media (Salonvaara et al 2006, Xu et al 2009, Rode et al 2020). The tests with gypsum wallboard, oriented strand board and silicate calcium using a dual chamber experimental system showed this similarity can be used to estimate the VOC diffusion coefficient if the water vapor diffusivity is known for the same material based on the conventional dry cup method (Salonvaara et al 2006, Xu et al 2009). Compared to the previous study of Xu et al (2009), the similarities between VOC and moisture transport in building materials have been extended for non-isothermal problems (Rode et al 2020, Tran Le et al 2021).

The use of vegetable particles (such as hemp shives, flax shives, straw bales, etc.) as building material aggregates is an interesting solution as they are eco-friendly materials. As the building materials represent an important part of indoor environments (hygrothermal comfort and IAQ), the purpose of this paper is to model and to investigate the similarities between VOC and moisture transport properties and and its impact on the indoor RH and VOC concentration for hemp concrete case. Hemp concrete is chosen for this study because it is more and more recommended by the eco-builders for its low environmental impact, excellent moisture buffering capacity and a good compromise between insulation and inertia materials (Collet 2008, Samri 2006, Tran Le et al 2010).

COUPLED HEAT, AIR, MOISTURE AND POLLUTANT TRANSPORT MODEL

A coupled Heat, Air, Moisture and Pollutant Simulation model dedicated to Bio-based materials called **CHAMPS-Bio** model (for non-isothermal and non-isobaric conditions) as presented in Figure 1 has been developed. This paper will focus only on the similarity between moisture and VOC transport models and the impact of the use of bio-based material (hemp concrete) on indoor air quality and hygric comfort.

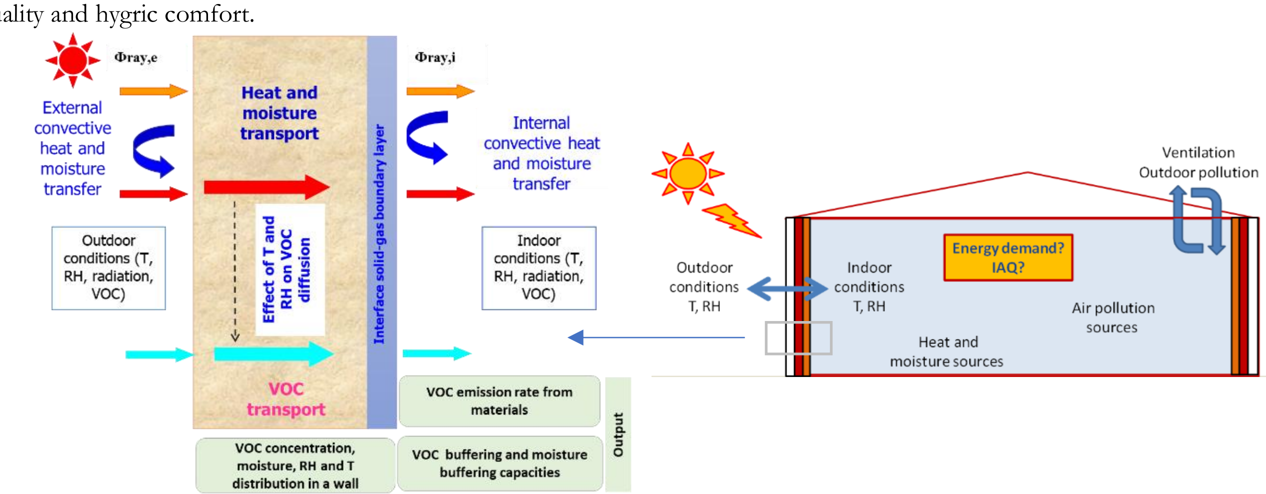

Figure 1: Schematic of coupled heat, air, moisture and pollutants transport model dedicated to Bio-based materials (**CHAMPS-Bio** model**)** in a wall and in a room developed and validated in the framework of Fulbright Project (Tran Le et al, 2021).

Similarity of pollutants and moisture transport models

In this article, the VOC and moisture diffusion models (that take into account the effect of moisture content in building materials on VOC transport if the data is available) are presented. To extablish the similarity between the VOC and moisture diffusion models, only concentration gradient of VOC or moisture is assumed to be driving force in the material. It is important to note that the chemical reactions are neglected in this work.

For a dry material with homogeneous diffusivity, the VOC mass transport within the wall can be described by the one-dimensional diffusion (Yang et al 2001, Huang and Haghighat 2002; Zhang 2005):

$$\frac{\partial C_{m,VOC}}{\partial t} = \frac{\partial}{\partial x}\left(D_{m,VOC} \frac{\partial C_{m,VOC}}{\partial x} \right) \quad (1)$$

Where $C_{m,VOC}$ is VOC concentration in the material (kg/m^3), $D_{m,VOC}$ is diffusion coefficient of the VOC in the material (m²/s), x is abscissa (m) and t is time (s). Here, in the developed numerical model, the $D_{m,VOC}$ is a function of relative humidity/moisture in the material (if the data is available) while the dependence of $D_{m,VOC}$ on pollutants concentration is neglected as generally accepted under low VOC concentration condition.

There is an equilibrium which exists between the concentration of VOC in a material ($C_{m,VOC}$) and the concentration in air ($C_{a,VOC}$), which is defined by the partition coefficient $K_{m,VOC}$:

$$C_{m,VOC} = K_{m,VOC} . C_{a,VOC} \quad (2)$$

The diffusion coefficient of VOC in the material ($D_{m,VOC}$) can be determined from the VOC diffusion coefficient in the free air (D_{VOC}^{air}) and diffusion resistance factor of VOC (μ_{VOC})(Xu et al 2009):

$$D_{m,VOC} = \frac{D_{VOC}^{air}}{\mu_{VOC} K_{m,VOC}} \quad (3)$$

At the material-air interface, we assume an instantaneous equilibrium between VOC concentration (kg/m^3) in the air near material surface ($C_{a,VOC,s}$) and the one in the surface layer ($C_{m,VOC,s}$):

$$C_{m,VOC,s} = K_{m,VOC} . C_{a,VOC,s} \quad (4)$$

With the following boundary conditions applied respectively for the external (x=0) and internal (x=L) surfaces of the wall:

$$-D_{m,VOC} \left. \frac{\partial C_{m,VOC}}{\partial x} \right|_{x=0,e} = h_{m,\mathrm{VOC},e} \left(C_{a,\mathrm{VOC},e} - C_{a,VOC,s,e} \right) \quad (5)$$

$$-D_{m,VOC} \left. \frac{\partial C_{m,VOC}}{\partial x} \right|_{x=L,i} = h_{m,\mathrm{VOC},i} \left(C_{a,VOC,s,i} - C_{a,\mathrm{VOC},i} \right) \quad (6)$$

Where $C_{a,VOC,i}$ and $C_{a,VOC,e}$ are VOC concentration in the room air and outside (kg/m^3), and $h_{m,VOC,e}$ and $h_{m,VOC,i}$ are convective VOC transfer coefficients (m/s) for the external and internal surfaces, respectively.

Concerning the moisture transport model, the moisture transport within the wall can be described by the one-dimensional diffusion for using moisture content in material as driving force (Philip and De Vries 1957):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left(D_{m,\mathrm{wv}} \frac{\partial \theta}{\partial x} \right) \quad (7)$$

Where θ is moisture content in the material (m^3 of water/m^3 of material), $D_{m,wv}$ is diffusion coefficient of the moisture in the material (m²/s) which is defined by:

$$D_{m,\mathrm{wv}} = \delta_{wv} \frac{P_{v,sat}}{\rho_w} \frac{1}{\partial\theta/\partial RH} = \frac{\delta_{wv}^{air}}{\mu_{wv}} \frac{P_{v,sat}}{\rho_w} \frac{1}{\partial\theta/\partial RH} \quad (8)$$

$\partial\theta/\partial RH$ is the slope of the sorption isotherm curve which designates the relationship between the moisture content and the relative humidity at a fixed temperature, δ_{wv} is water vapor permeability of material (kg/(m.s.Pa)), $P_{v,sat}$ saturation pressure of water vapor (Pa), μ_{wv} the vapor diffusion resistance factor and δ_{wv}^{a} is water vapor permeability of still air ((kg/(m.s.Pa)) which can be determined from D_{wv}^{air} (water vapor diffusion coefficient in the free air, m²/s), temperature and the gas constant for water vapor (R_v= 461.5 J/(kg·K)):

$$\delta_{wv}^{a} = \frac{D_{wv}^{air}}{R_v T} \quad (9)$$

By replacing (9) in (8) we have:

$$D_{m,\mathrm{wv}} = \frac{D_{wv}^{air}}{\mu_{wv} \dfrac{\rho_w R_v T}{P_{v,sat}} \dfrac{\partial\theta}{\partial RH}} = \frac{D_{wv}^{air}}{\mu_{wv} K_{m,wv}} \quad (10)$$

As with the VOC, by identifying two equation (3) and (10), the coefficient $K_{m,wv}$ introduced in (10) is the "partition coefficient" for water vapor, which is similar to $K_{m,VOC}$ in (3) for VOC and can be calculated as following:

$$K_{m,wv} = \frac{\rho_w R_v T}{P_{v,sat}} \frac{\partial \theta}{\partial RH} \tag{11}$$

Note that the partition coefficient (Km,wv) for water vapor can be introduced by relating gradients of the absorbed moisture content mass by volume of material, to gradients of the humidity of air by volume of the pores at equilibrium condition. Using this definition to calculate Km,wv, the same result was obtained (Rode et al 2020).

At the material-air interface, we assume an instantaneous equilibrium between water vapor concentration (kg/m^3) in the air near material surface ($C_{a,wv,s}$) and the one in the surface layer ($C_{m,wv,s}$), which is determined by the sorption isotherm curve. The following boundary conditions applied to water vapor, respectively for the external (x=0) and internal (x=L) surfaces of the wall:

$$-\rho_w D_{m,wv} \frac{\partial \theta}{\partial x}_{x=0,e} = h_{m,\mathrm{wv},e}\left(C_{a,\mathrm{wv},e} - C_{a,wv,s,e}\right) \tag{12}$$

$$-\rho_w D_{m,wv} \frac{\partial \theta}{\partial x}_{x=L,i} = h_{m,\mathrm{wv},i}\left(C_{a,wv,s,i} - C_{a,\mathrm{wv},i}\right) \tag{13}$$

Where $C_{a,wv,i}$ and $C_{a,wv,e}$ are water vapor concentrations in the room air and outside (kg/m^3), and $h_{m,wv,e}$ and $h_{m,wv,i}$ are convective water vapor transfer coefficients (m/s) for the external and internal surfaces.

Model for a room

In order to model the indoor VOC and humidity in the room, we used a nodal method, which considers the room as a perfectly mixed zone characterized by a moisture and pollutant concentrations. Nodal method involves equations for moisture/pollutant (VOC) mass balance and equations describing mass transfer through the walls, additional convection between inside wall surfaces and room ambiance. The moisture/VOC level in the room is determined by the moisture/VOC transfer from interior surfaces, moisture/VOC production rate and the gains or losses due to air infiltration, natural and mechanical ventilation, sources due to habitants of room as well as the moisture/VOC buffering capacity of other room elements (such as furniture, bookshelf, woolen carpet, etc.). This yields to the following mass balance equation for water vapor/VOC:

$$V\frac{\partial C_{a,i}}{\partial t} = Q\left(C_{a,o} - C_{a,i}\right) + \sum A.h_{m,i}\left(C_{as,i} - C_{a,i}\right) + G \tag{14}$$

Where $C_{a,i}$ is the VOC/water vapor concentration at time t (kg/m^3); $C_{a,o}$ is outdoor ventilation air; V is volume space (m^3); A is exposed area of the material (m^2), Q is the volume air flow rate into (and out) of the room (m^3/s), G is the generation rate of VOC/water vapor in the room (kg/s).

The set of equations describing the model has been solved using the finite difference technique with an implicit scheme. The Simulation Problem Analysis and Research Kernel (**SPARK**) developed by the Lawrence Berkeley National Laboratory-USA, a simulation environment allowing to solve efficiently differential equation systems has been used to solve this set of equations (Sowell and Haves 2001; Wurtz et al 2006; Mendonça et al 2006; Tran Le et al 2009; Tran Le et al 2016).

Note that the equations contain several parameters that are themselves function of the state variables. The special interests of the developed model in this paper are the dependencies of moisture transport coefficient, pollutant diffusion coefficient, partial coefficient, etc. upon the relative humidity and temperature can be taken into account if the data is avaiable. This makes it possible to take into account of the effect of T and RH on pollutant and hygrothermal behavior of building materials into the model. Concerning the model validation, the moisture model and pollutant models have been validated separately in previous articles (Tran Le et al 2016, 2021).

MODELLING VOC PROPERTIES FROM MOISTURE PROPERTIES OF HEMP CONCRETE

An increased environmental awareness incites to the valorization of plant resources as buildingmaterials or incorporating construction processes. One of these building materials is hemp concrete, which has been used widely in the world and extensively studied in many researches. At the building level, it has been proven that the use of hemp concrete can damping the variation indoor RH thank to its moisture buffering capacity (Tran Le et al 2010). Note that the composition and manufacturing have a significant impact on hygrothermal properties and anisotropie of hemp concrete. This article focuses on modelling VOC properties of sprayed hemp concrete which is made of hemp shiv mixed with a PF70 binder for wall application, from the moisture properties experimentally determined in (Collet et al 2013, Lelievre 2015, Colinart et al 2017). The toluene (TOL) was selected for this study as reference VOCs because it is a typical indoor VOC and not water soluble. Regarding the fact that the calculated mean free path for toluene is 14.3 nm (Xu et al 2009) and the mean pore diameter in hemp concrete is about 780 nm (Collet 2004), the molecular diffusion dominates the mechanism for toluene. Concerning water vapor, its mean free path is 100 nm (Collet 2004), the molecular diffusion is predominant in hemp concete compared to Knudsen diffusion which is also expected to occur.

Xu et al (2009) proposed the similarity coefficient to correlate the pore diffusion coefficient of VOCs with that of water vapor for hygroscopic moisture conditions in which open pore porosity does not change significantly. The similarity coefficient for the moisture and VOC can be determined by:

$$\kappa_{VOC} = \frac{\mu_{VOC}}{\mu_{wv}} = \frac{D_{VOC}^{air}}{\mu_{wv} D_{m,\mathrm{VOC}} K_{m,VOC}} \tag{15}$$

The partition coefficient of VOC can be determined based on the vapor pressure of the compound for different materials. Based on the data obtained by Bodalal (1999), the following correlation may be used when the material and compound to be studied do not match the data available (Yang et al 2001):

$$K_{m,VOC} = 10600 P^{-0.91} \tag{16}$$

where P is the vapor pressure of the compound in mmHg. By using equation (16) for toluene (P=25.8 mmHg at 23°C), the partition coefficient of toluene $K_{m,\mathrm{VOC}}$ for hemp concrete is 550.

The similarity coefficient between toluene and water vapor (κ_{VOC} =0.56) which was experimentally determined by Xu et al (2009) is used to estimate the VOC diffusion coefficient for hemp concrete in this study. Table 1 and Figure 2 show the physical properties, the vapor diffusion resistance factor and adsorption isotherm of hemp concrete obtained by other authors (Collet et al 2013, Colinart et al, 2017, Lelievre 2015). The results showed that hemp concrete is a very porous and hygrosopic material. The calculated values of $\mu_{m,\mathrm{VOC}}$ and $D_{m,\mathrm{VOC}}$ by equations (15) are shown in Table 2.

Concerning the partition coefficient of water vapor ($K_{m,wv}$), it is calculated by Equation (11) and the result determined at 10% RH is reported in Table 2. Equation (11) shows that $K_{m,wv}$ depends on temperature, relative humidity and the slope of the sorption isotherm of material. Note that it is very interesting to study the similarity ($K_{m,\mathrm{VOC}}$/ $K_{m,wv}$ and $\mu_{m,\mathrm{VOC}}$/ $\mu_{m,wv}$ for storage and diffusion properties, respectivelly) between VOC and moisture transport in material. If the similarity is justified and validated by experimental results, the VOC properties can be determined directly from the vapor diffusion resistance factor ($\mu_{m,wv}$) and the slope of the sorption curve in the monolayer sorption range (from 0 to 20% RH, before the beginning of multilayer sorption for hemp concrete case) because the VOCs sorption is generally monolayer in building materials. The experimental study on similarity between VOC and moisture transport in hemp concrete will be carried out in the future using the dual test chamber and will be discussed in another paper.

Table 1: Physical and hygric properties of hemp concrete to model VOC properties

	Dry density	Total porosity [%]	Open porosity [%]	μ_{wv}
Hemp concrete	450	78	66	5

Table 2: D_m and K_m for water and toluene of hemp concrete

	μ	K_m	D_m
Water vapor (wv)	5	1434 at 10% RH	3.1×10^{-9} (at 50% RH)
Toluene (VOC)	2.8	550	5.5×10^{-9}

EFFECT OF VOC AND MOISTURE BUFFERING CAPACITIES OF HEMP CONCRETE WALL ON INDOOR RELATIVE HUMIDITY AND VOC CONCENTRATION

Description of studied room and simulation conditions

The studied office is depicted in Figure 3 and has a space area of 5*4 m² and a volume of 50 m³. To study the impact of moisture and VOC buffering capacities of hemp concrete on the indoor RH and VOC concentration, we consider a total exposed surface area S=25 m² of hemp concrete (moisture and VOC interactions between indoor air and building materials are taken into account). The hygric and pollutant properties of hemp concrete presented in Table 1-2 and Figure 2 were used for the simulation. The room temperature is kept at 20°C. The outdoor temperature and relative humidity are 20°C and 50 %, respectively. The room is occupied by two persons from 8.00 am to 17.00 pm and the water vapor source is 142 g/h.

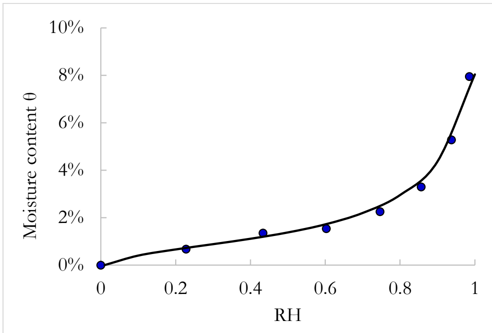

Figure 2: Sorption isotherm of hemp concrete

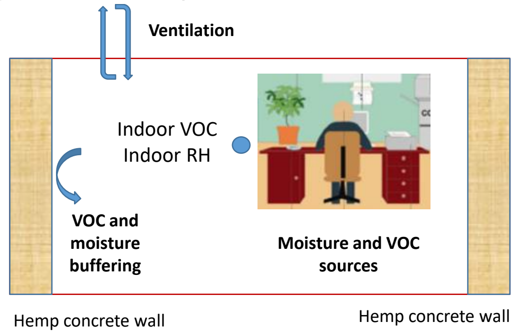

Figure 3: Studied configuration

In this article, an outdoor VOC (toluene) concentration of 0 mg/m³ and a ventilation rate of 0.72 ACH determined based on the ventilation rate required in the office buildings are considered. The hemp concrete wall has a thickness of 20 cm and is divided into 25 nodes. The time step is 240s. The only interaction (moisture/VOC) between the internal exposed surface of hemp concrete wall and indoor air is taken into account and the other faces of the material are considered "well sealed". The initial relative humidity is 60% RH and the initial VOC concentrations C_O in hemp concrete is 0 (μg/m³) because it is considered as a very clean material. To study the effect of VOC buffering capacity of hemp concrete, a toluene source scheme following is considered: 12 hours of 1000 μg/h followed intermittently 12 hours of 0 μg/h.

In this paper, two models have been considered:

- **Model with buffering capacity (BC** model**)**: Simulation taking into account the moisture and VOC sorption capacities (the room model is coupled to the wall model).
- **Model without buffering capacity (Without-BC** model**)**: Simulation neglecting the moisture and VOC sorption capacities (the room model is not coupled to the wall model).

Results and discussions

The simulated results of the two models with and without VOC-moisture buffering capacity are presented in Figure 4 and Figure 5. In addition, Table 3 presents the analysis results (indoor RH and TVOC concentration) obtained from the simulation when the equilibrium state is reached. Figure 4 showed a significant effect of the VOC buffering capacity of hemp concrete on indoor VOC variation. We define a parameter called "*peak reduced factor-PRF_{VOC}*" which is calculated from the indoor VOC concentration with and without VOC buffering capacity (C_0 corresponds to the case without VOC capacity): $PRF=(C_0-C)/C_0$. The PRF value allows to quantify the VOC buffering capacity of building materials. Regarding the values of indoor pollutant concentration at the equilibrium state, the maximum values of of **BC** and **Without-BC** models are 23.3 and 27.8 μg/m³, respectively (Table 3) (so a RF_{VOC} of 16%). Note that RF_{VOC} value depends on the exposure time. From IAQ analysis and design point of view, it is very interesting to define a parameter that takes into account the concentration reduction and exposure time. Thus, we define an indice called "Cumulative Exposure Reduction Factor, ERFc" (unity is %.h)" which is calculated by: $ERFc=\int_0^t PRFdt$; the ERFc is 210.5 % for 12 hours exposure in this study. The results reveal that taking into account the VOC sorption capacity in the simulation results in damping the peak of indoor VOC concentration and thus contributes to ameliorate the indoor air quality.

Concerning the variation of the indoor relative humidity, it is presented in Figure 5 and Table 3. The results showed that the moisture buffering capacity of hemp concrete allows to dampen the indoor relative humidity variation. Numerically, at the equilibrium state, the maximum indoor RH values decrease from 72.5 % to 66.5% RH (a difference of 6.2 % RH and PRF_{RH}=8.6 %) for **Without-BC** and **BC** models, respectively. For indoor humidity, we define a parameter called "*reduced factor-RF_{RH}*" which is calculated from the amplitude of indoor relative humidity variation with and without moisture buffering capacity (A_0 corresponds to the case without moisture capacity): $RF_{RH}=(A_0-A)/A_0$. The RF_{RH} value allows to quantify the hygric buffering capacity of building materials. In addition, a RF_{RH} value of 43.4 % is obtained showing that taking moisture buffering capacity into account can reduce the indoor RH variation amplitude by 43.4 %.

Table 3: Effect of VOC and moisture sorption capacity on indoor VOC concentration and RH calculated at the equilibrium state

	Indoor Toluene (μg/m³)			Indoor RH (%)		
	TOL min	TOL max	Amplitude	RH min	RH max	Amplitude
BC model	3.2	23.6	20.4	53.5	66.3	12.8
Without-BC model	0	27.8	27.8	50	72.5	22.5

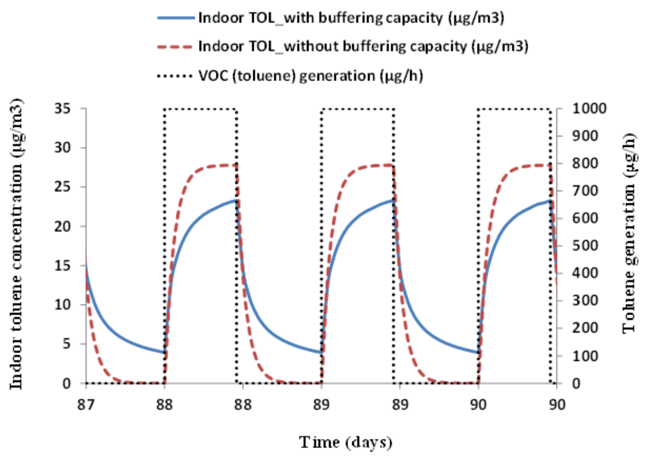

Figure 4: Effect of toluene sorption capacity on indoor toluene concentration

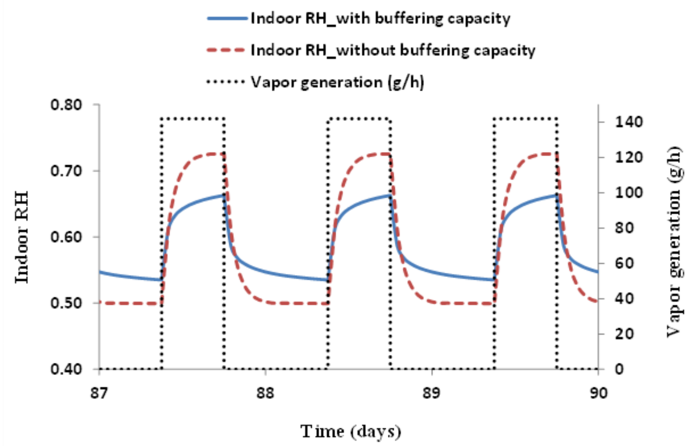

Figure 5: Effect of moisture sorption capacity of hemp concrete on indoor RH

CONCLUSION

In this paper, the similarity and the potential of VOC and moisture buffering capacities of hemp concrete on indoor air quality and hygric comfort has been modeled and investigated. The toluene properties ($K_{m,VOC}$ and $D_{m,VOC}$) were determined from the hygric properties of hemp concrete based on the assumption of the similarity between the moisture and pollutant transport in porous materials. The moisture and VOC transport models have been compared and implemented in SPARK, an object-oriented program suited to complex problems. The numerical model was applied to investigate the effect of the VOC and moisture buffering capacities of hemp concrete on indoor VOC concentration and relative humidity. The results reveal that taking into account the sorption capacity toward moisture and VOC of hemp concrete has a significant impact on hygric comfort and indoor air quality. Numerically, in this case studied, hemp concete can contribute to dampen 16% indoor VOC concentration and 43.4 % indoor RH variation amplitude. In addition, indices are also proposed to represent the buffering capacity of materials in reducing the occupant's peak exposure and cumulative exposure to VOCs. The definitions are useful for consideration in future standards that consider buffering as an approach to improving IAQ as well as hygrothermal performance of buildings. Finally, it is important to note that the developed numerical model can predict the entire emission life of the material to overcome the measurement difficulties.

ACKNOWLEDGMENTS

This study was carried out within the project **CHAMPS-Bio** under the programe Fulbright /Hauts-de-France which is supported by Hauts-de-France region and the Franco-American Fulbright Commission. The authors wish to thank them.

NOMENCLATURE

D_m	Mass transport coefficient associated to a moisture content or VOC gradient	$m^2.s^{-1}$

K Partition coeficient

Subscripts

e= external *m*= material *i*= internal w=water w*v*= *water vapor*

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