



Smart materials for energy efficient IAQ management



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ANNEX 86

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1



Time	Activity
14:00	Welcome and introduction Menghao Qin – DTU, DK
14:10	Metal-organic Frameworks for indoor environment control Menghao Qin – DTU, DK
14:30	Passive Removal Materials for Indoor Air Improvement: Performance Evaluation and Modeling Doyun Won & Mitra Bahri – NRC, CA
14:50	Electrospun fibers for Supply Air Filtration in residential buildings, Alireza Afshari – AAU, DK
15:10	Impact of VOC and moisture buffering capacities of bio-based building materials on IAQ and indoor RH: the case of hemp concrete Anh Dung TRAN LE –UPIJV, FR
15.30	Discussion Jensen Zhang – SU, USA
15.45	End of meeting

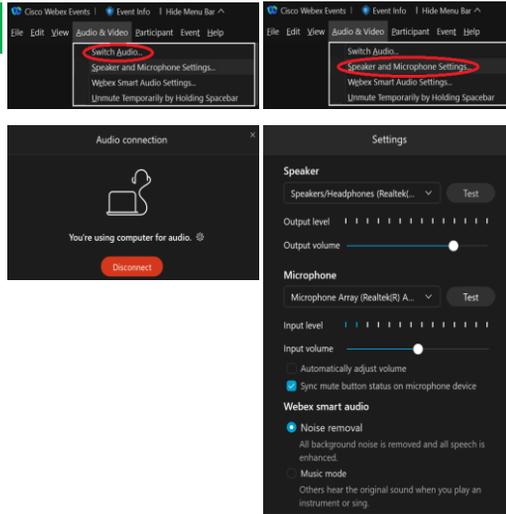
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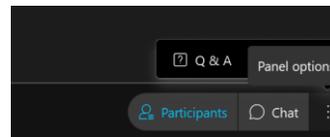
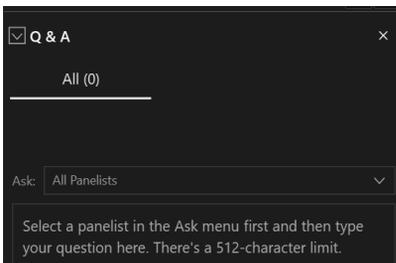
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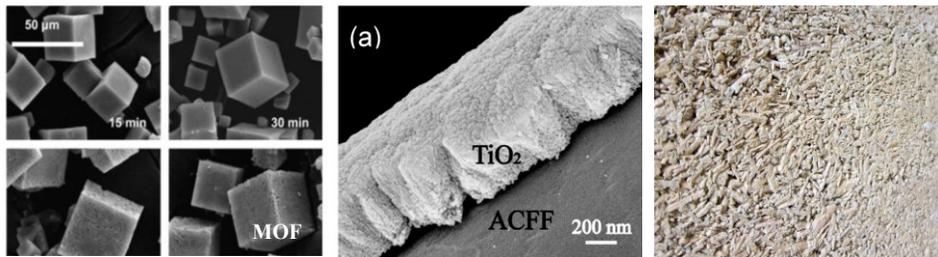
IEA Annex 86 Subtask 3

Smart materials as an IAQ management strategy

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General description

- ST 3 identifies opportunities to use novel materials (from advanced functional nano-materials to bio-based building materials) as building components to actively/passively manage the IAQ, for example, through active paint, wallboards and textiles coated with advanced sorbents or catalysts and quantify their potential based on the assessment framework developed in ST 1.



Activities

• A3.1 Material properties and characterization of the products

Literature survey and laboratory testing to gather relevant data and existing knowledge about properties for transport, retention, and adsorption of chemical substances and moisture in new functional materials (e.g. Metal-organic frameworks (MOFs), photo-catalysts, precise humidity control material (PHCM), hemp concrete, etc.). The synergistic effect of VOC and moisture on the removal performance of the new materials will be studied.

• A3.2 Modelling of the behaviour under typical residential conditions

Model setup and laboratory tests to analyse the performance of the new materials for IAQ control in residential buildings. The behaviour of the materials over time under different climates will be analysed and corresponding control strategies for IAQ management will be developed.

• A3.3 Assessing energy-saving and exposure reduction potential

Numerical simulations to study the energy-saving and exposure reduction potential of the new smart materials in residential buildings under different climatic conditions.

• Stakeholders involved:

- Manufacturers of building materials shall be involved regarding testing and possible co-development of products that have a function to absorb indoor pollutants.
- Building designers, health organizations, and technological institutes who make testing for industry and run their labelling systems are also among potential stakeholders.

• Deliverables:

- D3.1 A comprehensive review of ad/desorption and transport properties of the smart materials developed in the project for IAQ control.
- D3.2 Mechanistic models for estimating the energy-saving and exposure reduction potential of the new materials under realistic environmental conditions. The data and models will be published in scientific journal articles and a project report.
- D3.3 A test method for evaluating VOC removal performance of the new materials under a realistic built environment.

Participants



AAU (DK), Aalborg University
BBRI (BE), Belgian Building Research Institute
BUCEA (CN), Beijing University of Civil Engineering and Architecture
CSIRO (AU), Commonwealth Scientific and Industrial Research Organisation
DTU (DK), Technical University of Denmark
ESPCI (FR), ESPCI Paris - PSL University
GU (BE), Ghent University
IPV-FEUP (PT), Polytechnic Institute of Viseu (IPV) and University of Porto (FEUP)
KUL (BE), KU Leuven
LBNL (USA), Lawrence Berkeley National Laboratory
MatNova (BE), Material Nova
NJU (CN), Nanjing University
NRC (CA), National Research Council
SJTU (CN), Shanghai Jiao Tong University
SU (USA), Syracuse University
TJU (CN), Tianjin University
TU/e (NL), Eindhoven University of Technology
UPJV (FR), University of Picardie Jules Verne

Metal-organic Frameworks (MOFs) for indoor environment control

Menghao Qin

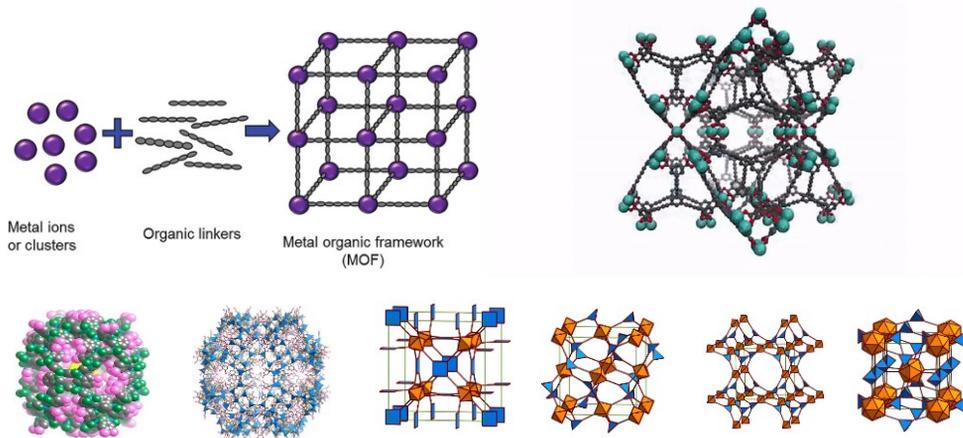
Technical University of Denmark (DTU)

AIVC & IEA EBC Annex 86 Joint Webinar
12 October 2021

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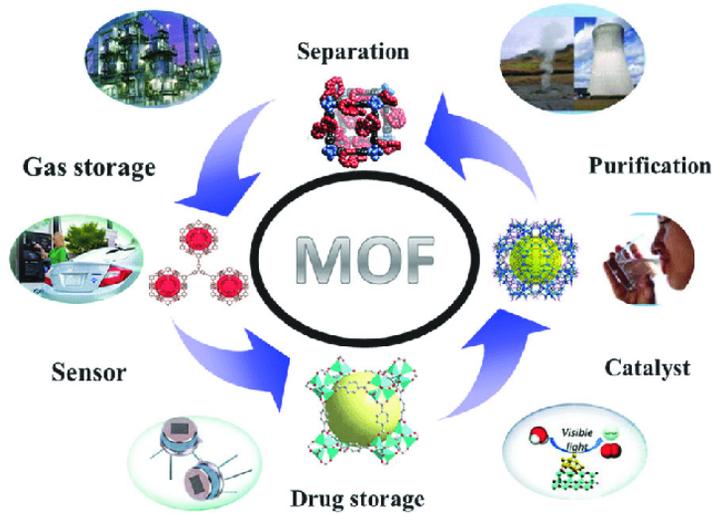
What is Metal-Organic Framework (MOF)?

- Metal-organic frameworks (MOFs) are a new class of organic-inorganic hybrid crystalline porous material.



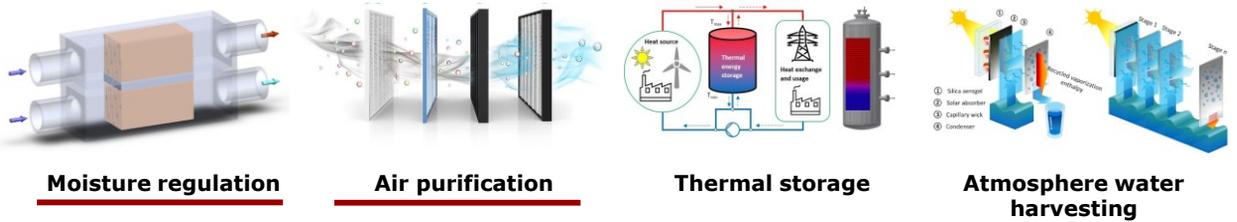
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Applications of MOFs



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MOFs applications in built environment



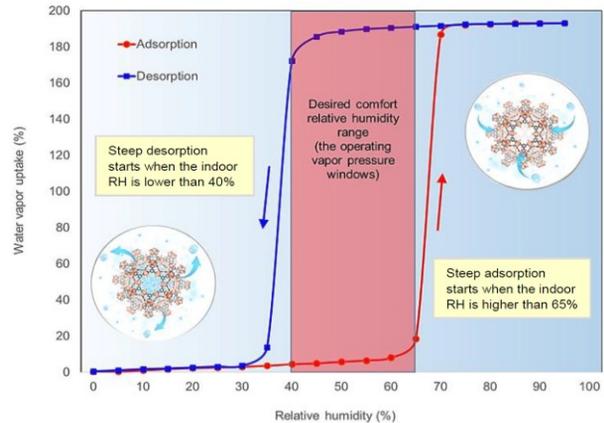
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App 1. MOF based autonomous humidity control materials

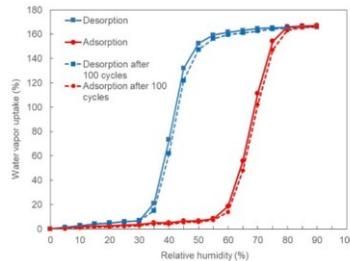
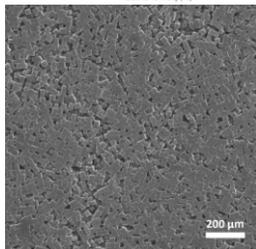
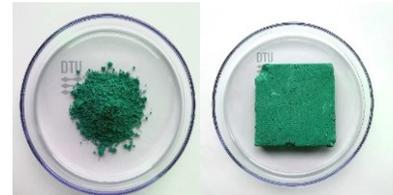
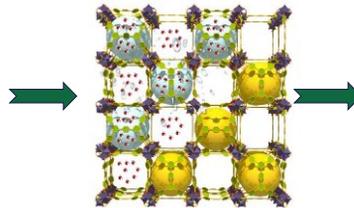
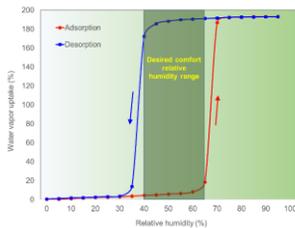
- Indoor relative humidity is an important parameter to determine indoor air quality, occupants' thermal comfort and building energy consumption. As recommended by ASHRAE, the appropriate indoor relative humidity range for indoor environment is **between 40% and 65% RH**.

The ideal materials for autonomous regulation of indoor RH should meet the following criteria:

- The material should have an S-shape isotherm and exhibit a steep uptake isotherm at a specific relative humidity depending on the targeted application.
- High water vapor uptake within the operating vapor pressure window;
- Low regeneration temperature and high reproducible cycling performance;
- High hygrothermal stability, non-toxicity and non-corrosion.



App 1. MOF based autonomous humidity control materials



MBV of MOF-PHCM is $20.50 \text{ g}\cdot\text{m}^{-2}\cdot\text{RH}^{-1}$ at 8 hours in the experimental conditions, which is almost **45** times higher than that of laminated wood and **36** times higher than gypsum

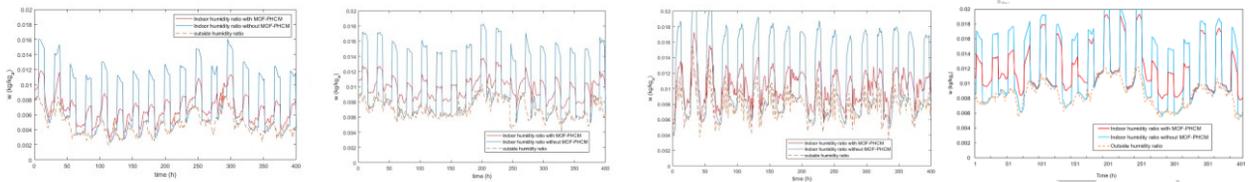
M. QIN et al, Precise humidity control materials for autonomous regulation of indoor moisture, Building and Environment, Vol. 169, 2020.

App 1. MOF based autonomous humidity control materials



Test and simulations in different climates

- Salt Lake City (semi-arid climate),
- Phoenix (hot desert climate),
- Paris (temperate climate),
- Madrid (moderate Mediterranean climate),
- Shanghai (humid subtropical climate).



M. QIN et al, *Precise humidity control materials for autonomous regulation of indoor moisture*, *Building and Environment*, Vol. 169, 2020.

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App 1. MOF based autonomous humidity control materials

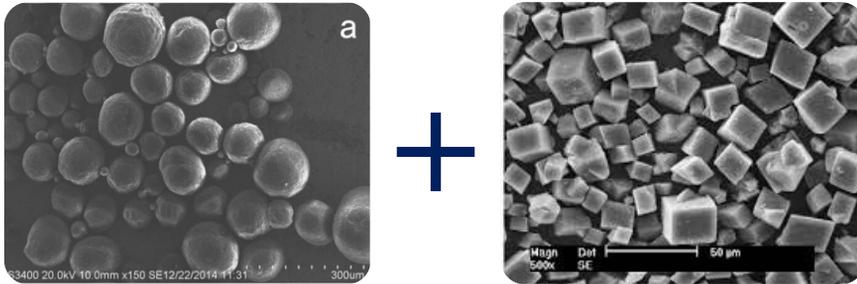
- MOF-PHCM can autonomously control indoor relative humidity within the thermal comfort range and reduce building energy consumption in most climates without any additional energy input.
- MOF-PHCM can be easily regenerated by either night ventilation (e.g. in hot desert, semi-arid, Mediterranean climates) or heating system powered by low-grade energy (e.g. in humid climates).



M. QIN et al, *Precise humidity control materials for autonomous regulation of indoor moisture*, *Building and Environment*, Vol. 169, 2020.

App 2. Metal-Organic Framework /Microencapsulated Phase Change Material Composites

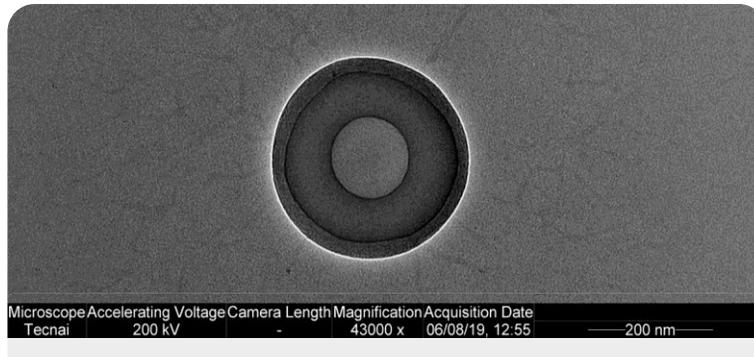
Phase Change Humidity Control Material (PCHCM) can moderate both the indoor temperature and moisture.



M QIN et al., Phase change humidity control material and its impact on building energy consumption. *Energy and Buildings* 174 (2018) 254-261.

App 2. Metal-Organic Framework /Microencapsulated Phase Change Material Composites

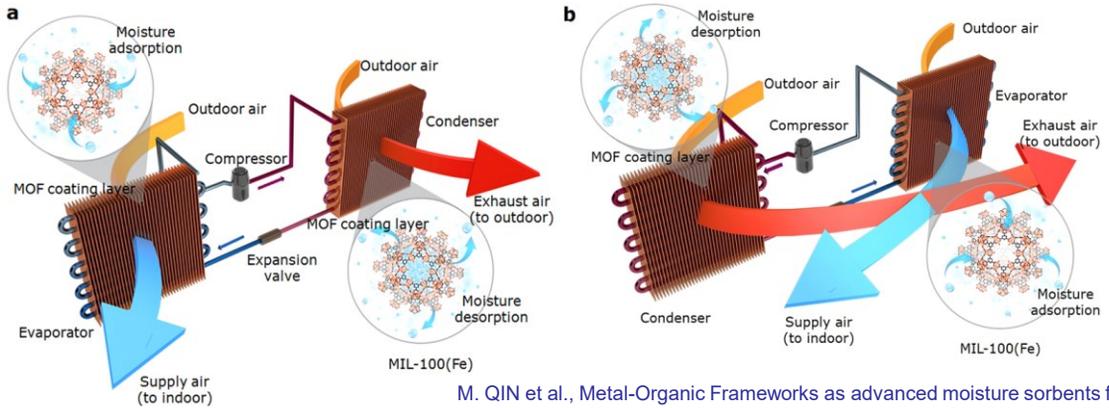
Double shell MOF/PCM composites can moderate both the indoor temperature and moisture. (2020)



M QIN et al., Preparation and Characterization of Metal-Organic Framework /Microencapsulated Phase Change Material Composites for Indoor Hygrothermal Control. *Journal of Building Engineering*, 2020.

App 3. MOF coated heat exchangers

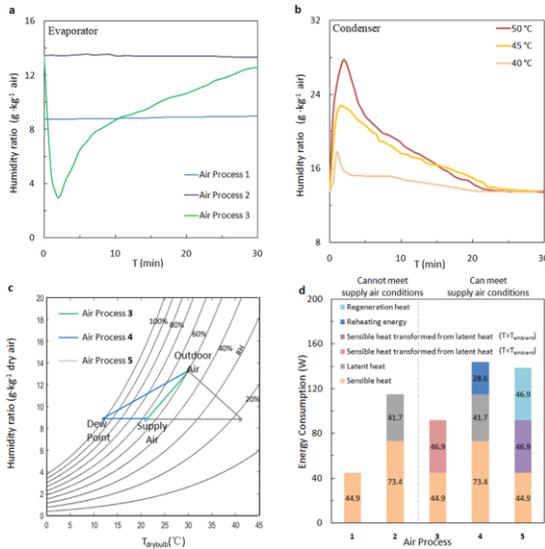
- Traditional vapour-compression air-conditioning has a low coefficient of performance (COP) due to the refrigeration dehumidification process, which often makes necessary a great deal of subsequent re-heating.



M. QIN et al., Metal-Organic Frameworks as advanced moisture sorbents for energy-efficient high temperature cooling, *Nature Sci. Rep.*, Oct. 2018.

13

App 3. MOF coated heat exchangers



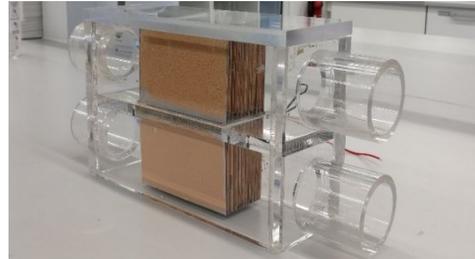
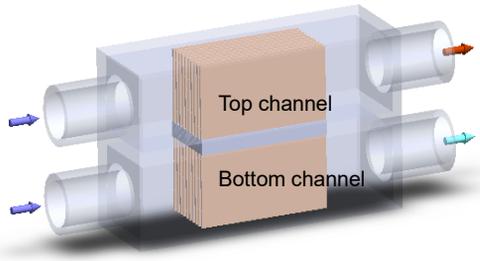
- MOFs coated heat exchangers has a good performance in removing **both latent and sensible heat loads simultaneously**.
- The system makes possible an energy-efficient working cycle with a **small temperature difference of less than 30 C** between the evaporator and the condenser
- The system **eliminates 36.1% of the working load** in refrigeration-based dehumidification by a conventional air-conditioner with reheating. The **overall COP of the system could be up to 7.9**.

M. QIN et al., Metal-Organic Frameworks as advanced moisture sorbents for energy-efficient high temperature cooling, *Nature Sci. Rep.*, Oct. 2018.

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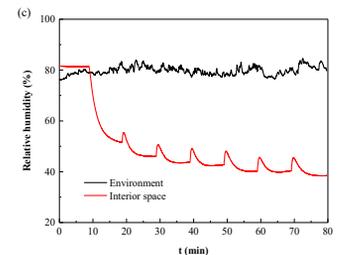
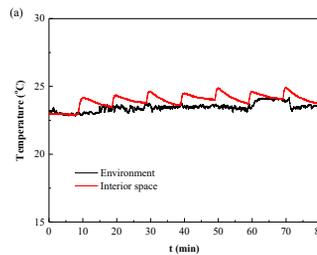
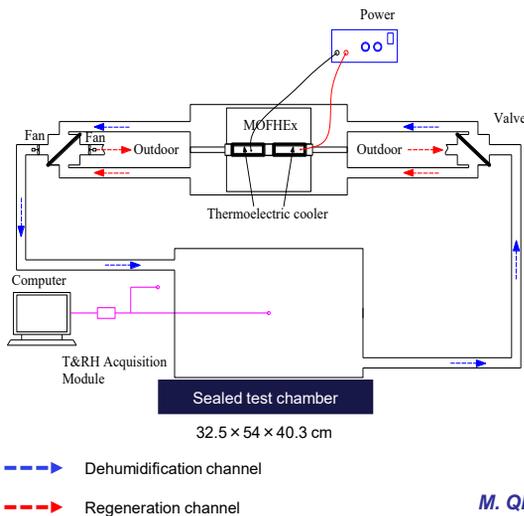
App 4. MOF humidity pump

The concept of a humidity pump is inspired by a heat pump. A humidity pump is a device that can transport moisture through the inverse gradient of vapor concentration, i.e., the vapor can be transferred from a relatively low-humidity space to a high-humidity space. For example, in summers, the humidity pump will transfer moisture from cool and less-humid indoor condition to a hot and humid outdoor condition; vice versa, in winters.



M. QIN et al., A novel metal-organic frameworks based humidity pump for indoor moisture control, *Building and Environment*, 107396, 2020

App 4. MOF humidity pump

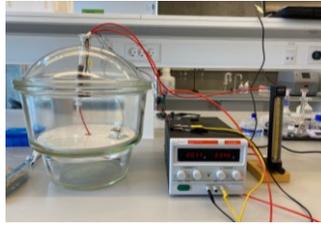
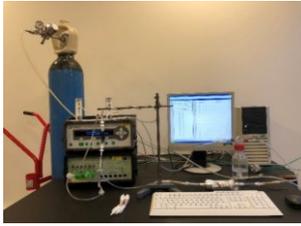
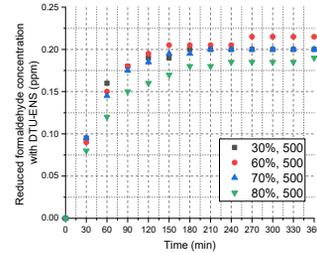
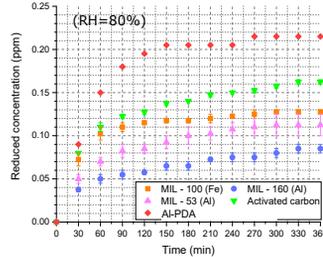


- *MOFs* are promising desiccants to the indoor environment control;
- The humidity pump can achieve dehumidification above the dew point temperature, improving the *overall efficiency*;
- The humidity pump has a *fast response rate* to the humidity load of a localized space;
- The humidity pump has *compact and flexible structures*.

M. QIN et al., A novel metal-organic frameworks based humidity pump for indoor moisture control, *Building and Environment*, 107396, 2020

App 5. MOFs for VOC (formaldehyde) removal

The DTU test conditions:
 temperature (23°C),
 Relative humidity (30%, 60%,
 70%, and 80%RH).
 The initial formaldehyde
 concentration is 0.26ppm



S. Chen, Master thesis, 2021

Conclusion

- MOFs with large adsorption capacity, the energy demand of desorption, ad/desorption kinetics, and cycling durability are good candidates for energy-efficient indoor environment control.
- Superior moisture sorption based on materials with enhanced water affinity, large surface area and high porosity can increase the water uptake to adsorb more moisture from the indoor air.
- Pyrazole-based MOFs are the best sorbents for FA adsorption from air.
- Low regeneration energy demand can be achieved by tailoring the sorption behavior of materials and incorporating functional materials,
- Fast moisture/VOC adsorption and desorption are essential for energy-efficient dehumidification/air cleaning within a short period of time.

Thank you for your attention!

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Passive Removal Materials for Indoor Air Improvement Performance Evaluation and Modeling

Doyun Won and Mitra Bahri

Indoor Air Quality (IAQ) Group, Construction Research Center
National Research Council Canada (NRC)
Ottawa, Canada



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Introduction

What are “Indoor passive removal materials (PRMs)”

- Building & coating materials, designed to improve IAQ with no or little energy input
- Gypsum boards, acoustic ceiling tiles, ceramic tiles, wallpapers & paints (based on sorptive or photocatalytic oxidation process)

Motivation

- Little information available for their performance
- Test in a standardized manner (chamber)
- Test in a room or house-scale

NRC Projects

- Controlled chamber test (Zuraimi Sultan, Bob Magee & Mitra Bahri)
- Research house test (Doyun Won and Mitra Bahri)
- Modeling (Mitra Bahri)

2

Facilities at NRC used for Evaluating Passive Removal Products

Environmental Chamber (400-L)

- ❑ Controlled for temperature, RH and air flow



Indoor Air Research Laboratory (IARL)

- ❑ Two rooms (side-by-side room test)



Semi-detached Twin Research Houses

- ❑ Two houses (side-by-side house comparison)



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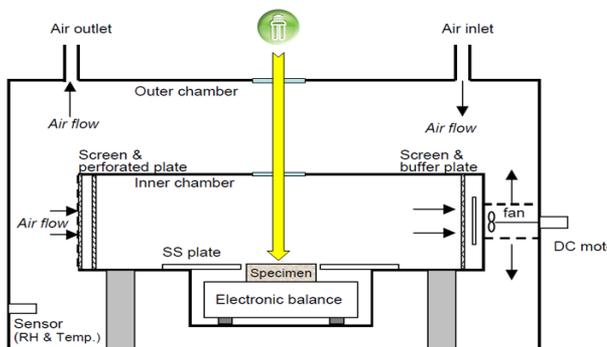
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Topic 1: 400-L Chamber Tests of Passive Removal Materials for IAQ

Objective: Evaluation of removal efficiency of passive removal materials

- ❑ 8 sorptive (gypsum board; ceiling tile; ceramic tile; wallpaper): normal vs. painted
- ❑ 3 photocatalytic oxidation (flooring; wallpaper; fabric): UV vs. visible light

Outcome: Test protocol



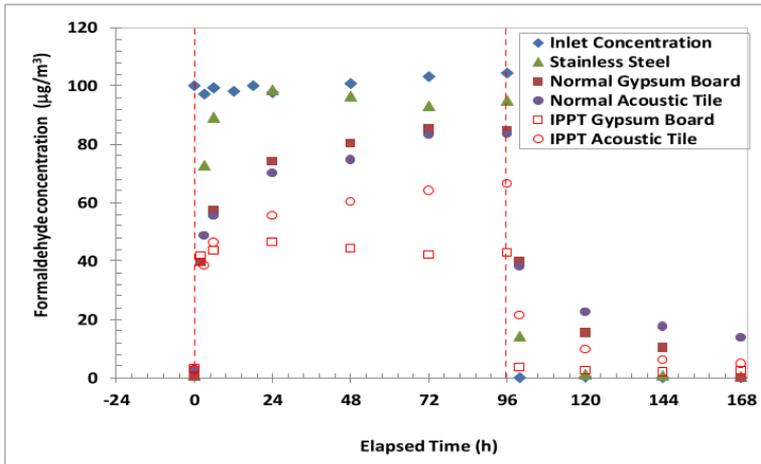
Standard conditions:

- $0.23 \text{ m}^2/\text{m}^3$
- 0.5 per hour
- $23 \pm 2 \text{ }^\circ\text{C}$
- $50 \pm 5\% \text{ RH}$
- 4 days + 3 days
- $1000 \pm 100 \text{ lx}$ or $14 \pm 3 \text{ W/m}^2$
- Formaldehyde or toluene

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Topic 1: 400-L Chamber Tests of Sorptive Passive Panel Technologies (Results)



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Removal Rate at Time t:

$$RR_A = (C_{i,t} - C_{o,t}) Q / A$$

$$VR_A = (C_{i,t} / C_{o,t} - 1) Q / A$$

Removal Rate Coefficient:

$$V \frac{dC_o}{dt} = Q \cdot C_i - Q \cdot C_o - k_{ss} \cdot A_{ss} \cdot C_o - k_p \cdot A_p \cdot C_o$$

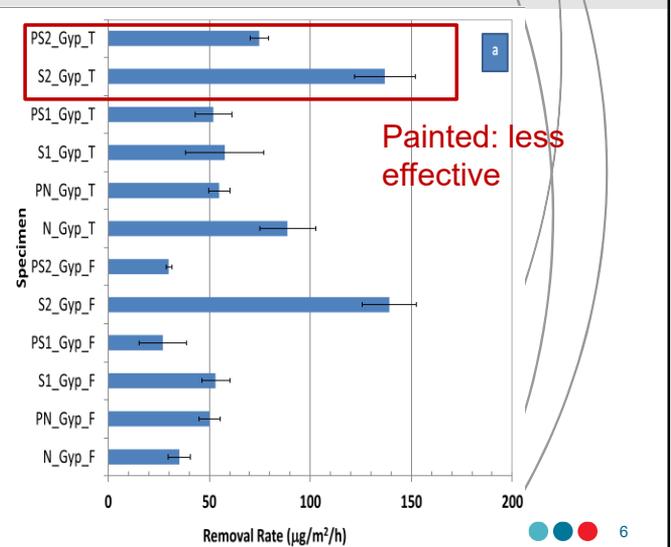
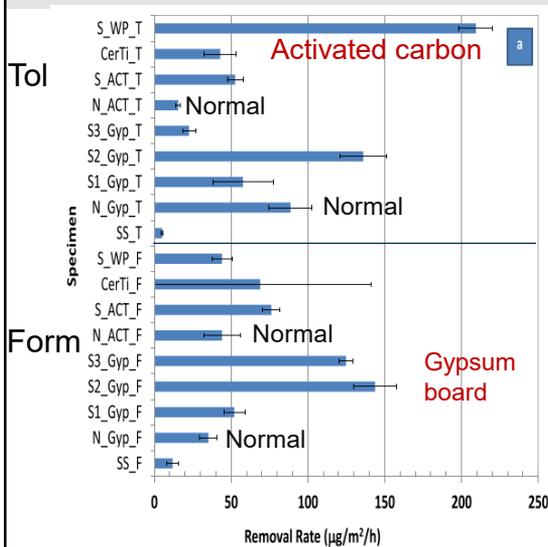
Stainless Chamber

Passive Panel

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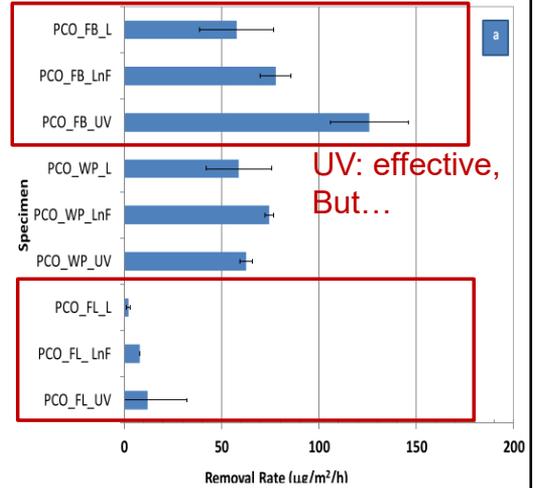
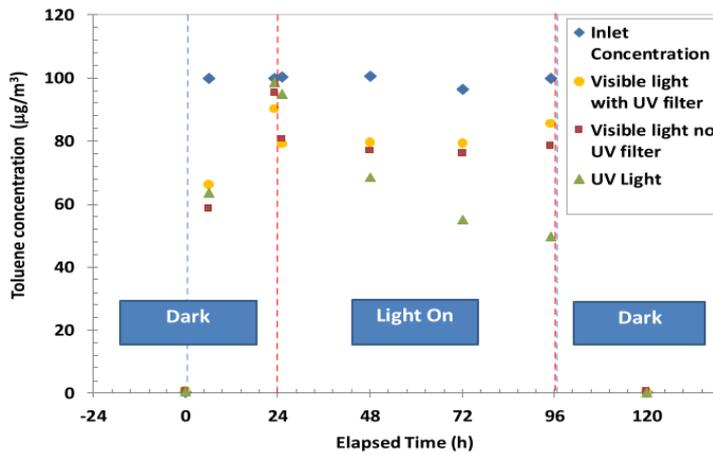
Topic 1: 400-L Chamber Tests of Sorptive Panel Technologies (Results: Removal Rate)



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Topic 1: 400-L Chamber Tests of PCO Passive Panel Technologies (Results)



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Topic 2: Research House Test (Drywall with “formaldehyde scrubbing” feature)

Unit E
East
(Structural materials treated w/ coating)



Unit F
West
(gypsum board, passive panel)

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Topic 2: Research House Test IAQ & Vent at 3 & 8 months (7-day, passive)



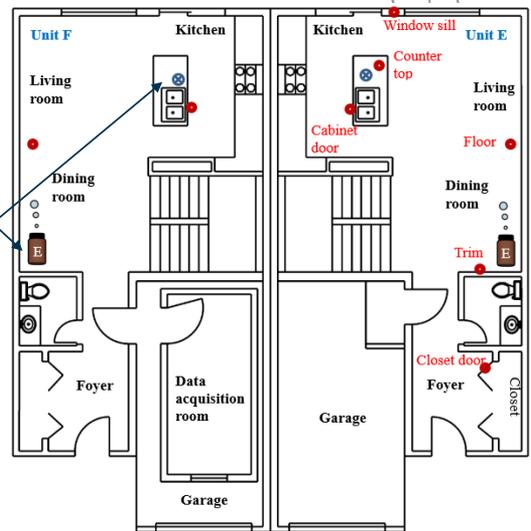
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Topic 2: Research House Test Ventilation Measurements using Perfluoro-carbon Tracer

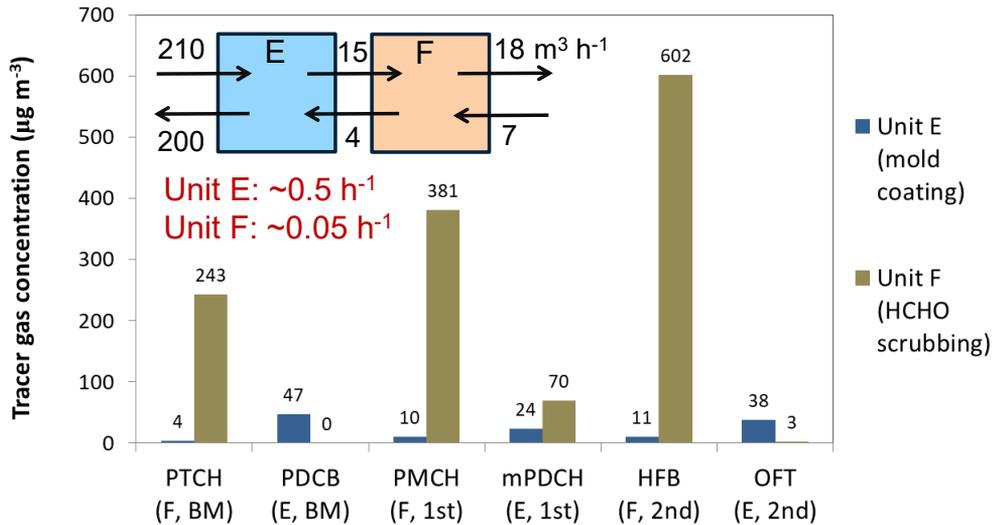
Unit E, East 2nd (OFT)	Unit F, West 2nd (HFB)
1st (mPDCH)	1st (PMCH)
BM (PDCB)	BM (PTCH)



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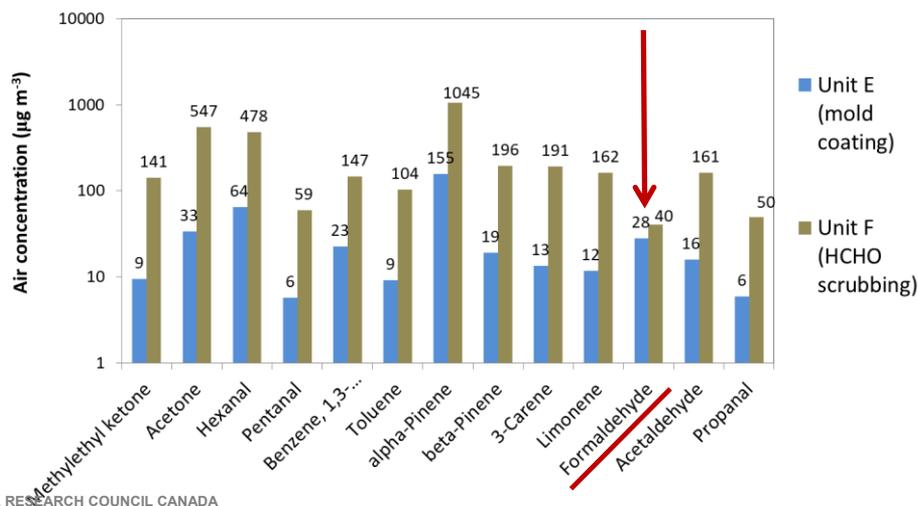
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Topic 2: Research House Test Conc. of Tracer Gases & Ventilation Rate



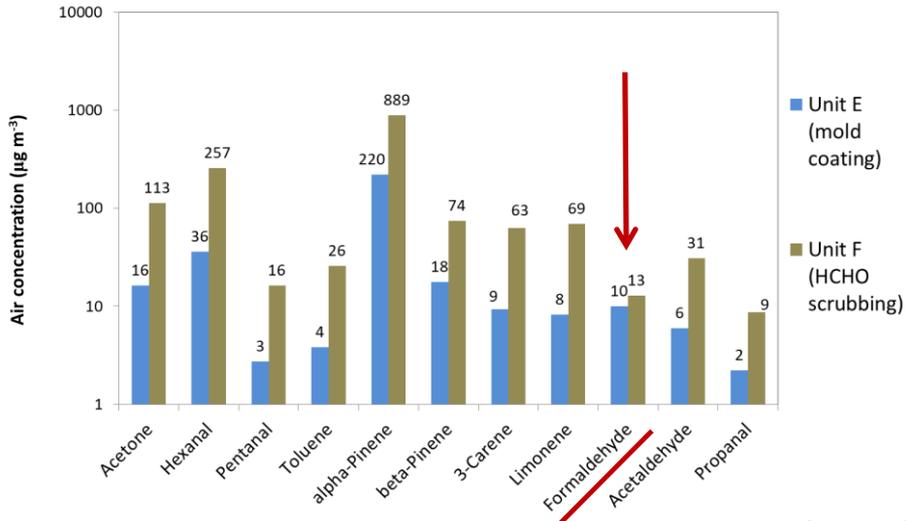
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Topic 2: Research House Test (VOC and HCHO concentrations @ 3 months)



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Topic 2: Research House Test (VOC and HCHO concentrations @ 8 months)



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Topic 2: Research House Test (drywalls decreased HCHO level by 3 – 4 times?)

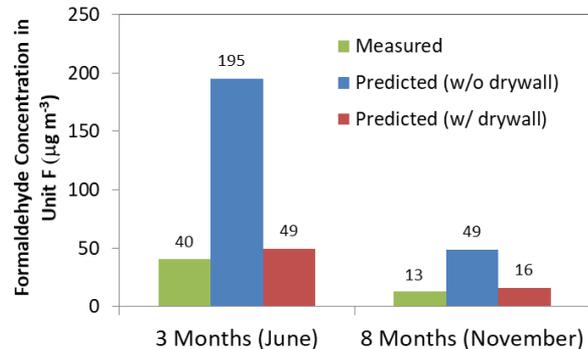
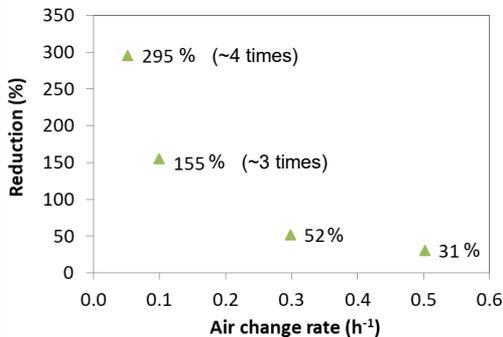
$$C_{indoor} = \frac{C_{outdoor} + \frac{\sum_{i=1}^n A_i \cdot EF_i}{Q}}{1 + \frac{k_p \cdot A_p}{Q}}$$

1st order removal by drywall

$$K_p = 0.2 \text{ m h}^{-1}$$

$$A_p = 323 \text{ m}^2$$

$$K_p \cdot A_p / Q = 3$$



14

14

Topic 3: Modeling

Experimental measurement

- **Advantage:** reliable research method, adequately describes the system and provides practical information
- **Disadvantage:**
 - lab-scale: mostly unrealistic condition
 - full-scale: expensive, time-consuming

Alternative approach: Simulation of indoor air environment

- Computational fluid dynamics (CFD): a powerful simulation tool to understand
 - concentration distribution, material performance, environmental effect, ...

Topic 3: Modeling

Modeling

Phase I : experiment & model

Phase II : experiment & model

Samples [2,3]

- Photocatalytic-based PRMs (3 Samples)
- Sorptive-based PRMs (8 Samples)

Performance Evaluation[2,3]

- Pollutant removal efficiency
- By-product formation
- Effect of environmental conditions
- The highest removal efficiency : a ceiling tile with ($\eta_r \sim 40\%-71\%$) [3]



400-L Test Chamber

$C_f = 100 \mu\text{g}/\text{m}^3$
 $T: (21^\circ\text{C} - 26^\circ\text{C}) \pm 2^\circ\text{C}$
 $\text{RH}: (30\%, 50\%, 75\%) \pm 5\%$
 $V_{\text{Air}}: 0.2 \text{ m}^3/\text{h}^{-1}, R: 0.5 \text{ h}^{-1}$
 $L_f = 0.23 \text{ m}^2/\text{m}^3$

Test duration 1: 7 days - 4 days sorp., 3 days desorp.
Test duration 2 = 28 days - 21 days sorp., 7 days desorp.

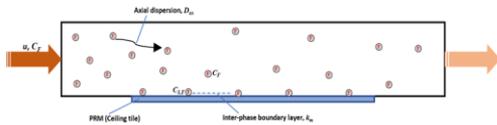


Topic 3: Modeling Methodology

Phase I:

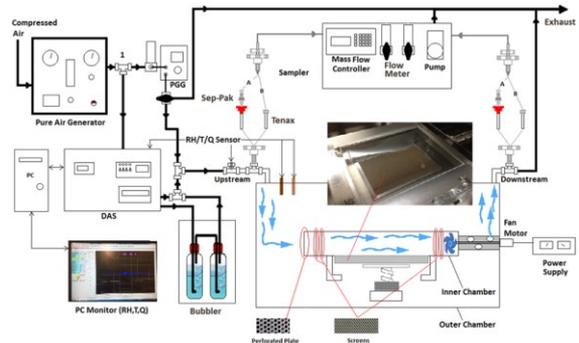
- PRM's formaldehyde removal performance evaluation in 400-L chamber
- Develop a model to find the sorption characteristics of PRM as a function of operational parameters

Modeling of the test chamber:
1-D mathematical model: Solved using MATLAB



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Schematic of the environmental test chamber (400 L)



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17

Topic 3: Modeling Indoor Air Research Laboratory (IARL)

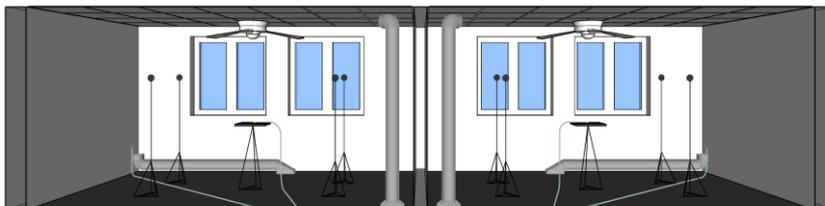
Phase II:

- The results is used for the development a CFD model – using COMSOL.



Sorptive Ceiling Tile

Standard Ceiling Tile



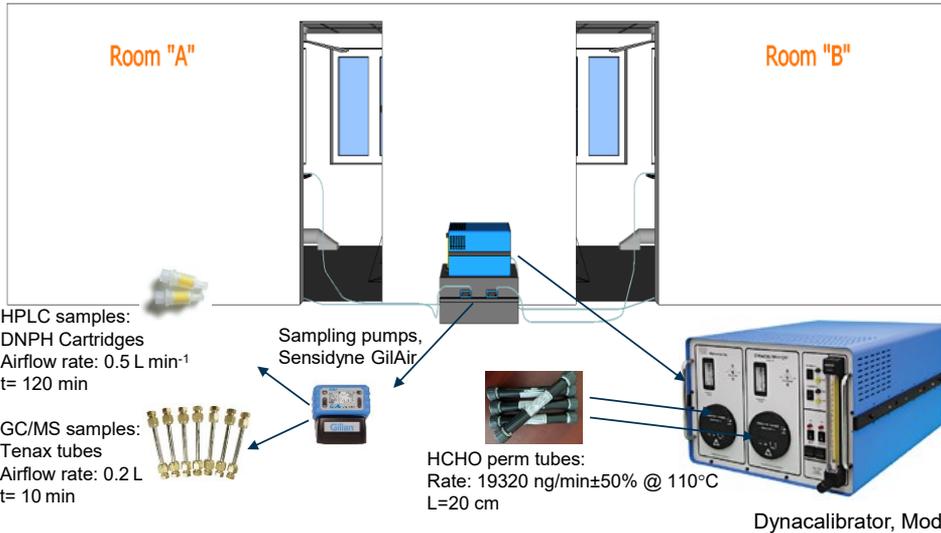
Two side-by-side test rooms ~ identical
Room Size:
H: 2.16 m (original: 3.05 m)
W: 2.41 m
L: 4.34 m
V_{Total}: 22.6 m³

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18

18

Topic 3: Modeling Methodology



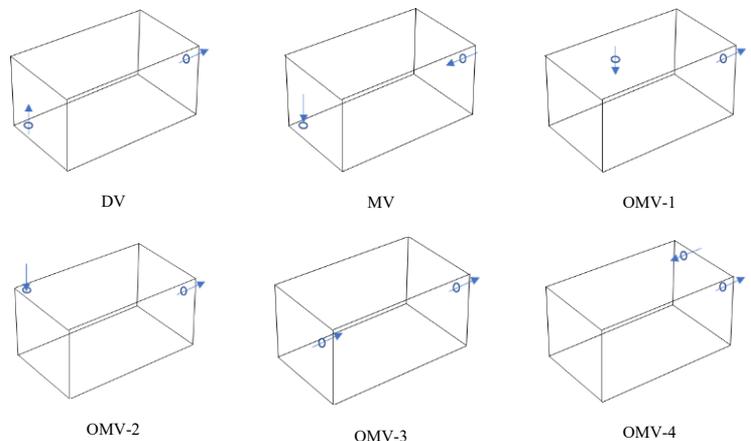
Topic 3: Modeling

CFD Modeling - Test Room

Model validation based on the SF₆ injection data (60cc/10 secs, DV)

Effect of different ventilation patterns on formaldehyde concentration distribution with and without PRM

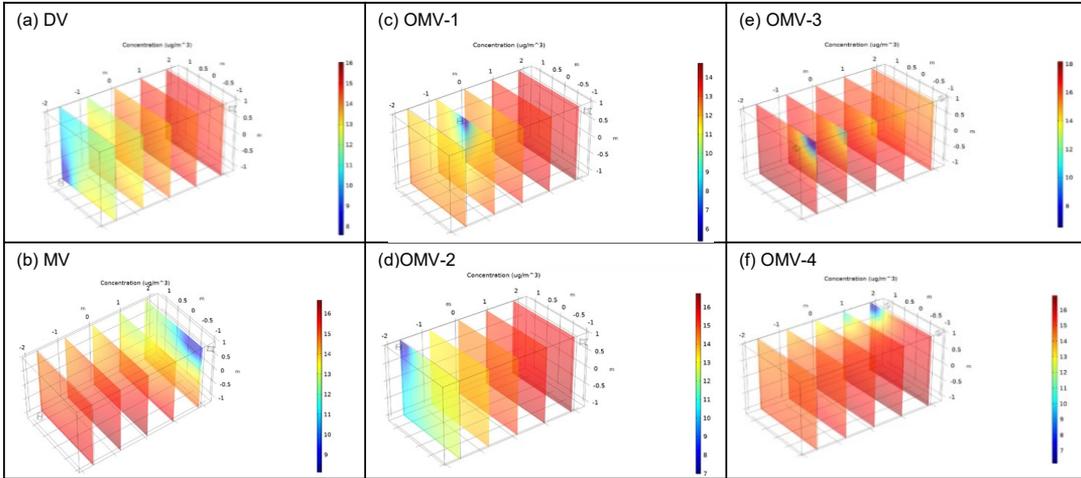
Formaldehyde emission source:
a wooden flooring (Birch)
emission rate: 49 µg.m⁻².h⁻¹



DV: Displacement ventilation
MV: Mixing ventilation
OMV: Over-headed mixing ventilation

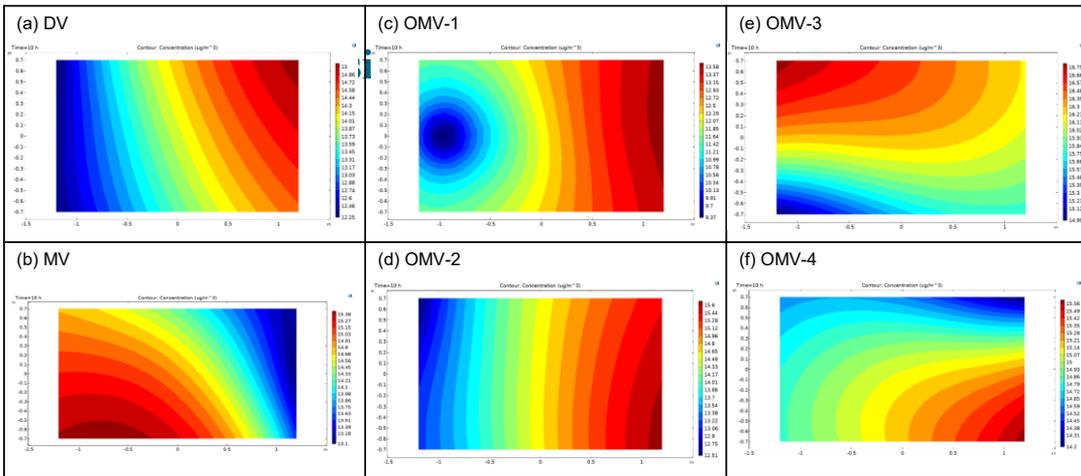
Topic 3: Modeling

Concentration profile in the test room



Topic 3: Modeling

Concentration profile in the breathing zone



Topic 3: Modeling Results

Effect of presence of PRM

Ventilation Pattern	DV	MV	OMV-1	OMV-2	OMV-3	OMV-4
Ave. conc. in BZ ($\mu\text{g}/\text{m}^3$) without PRM	13.8	14.6	12.1	14.5	16.2	15.0
Ave. conc. in BZ ($\mu\text{g}/\text{m}^3$) with PRM	9.8	10.2	8.8	10.0	11.0	10.3
% Of improvement	41.7	44.0	38.4	44.4	47.2	45.9

Topic 3: Modeling Results

Health-risk assessment (HRI)

$$HRI = \sum \frac{C_F}{REL_F}$$

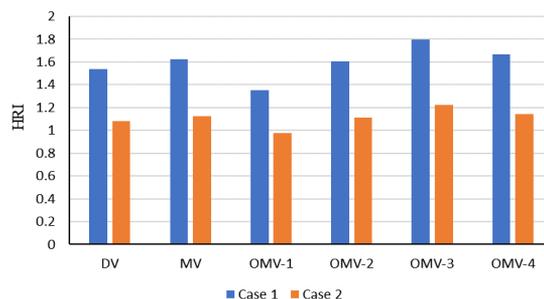
• REL_F : recommended exposure limit

- NIOSH recommendation: $19.5 \mu\text{g}/\text{m}^3$
- OEHHA recommendation: $9.0 \mu\text{g}/\text{m}^3$

• Formaldehyde Conc. falls into safe levels in the presence of PRM

• PRM: a potential replacement method for IAQ improvement and energy saving in built environments

Effect of presence of PRM



Future plan

- Re-visit side-by-side test houses under realistic conditions ($< 0.2 \text{ h}^{-1}$)
- Develop the model, estimate the PRMs life-time, effect of environmental condition (T,H), presence of mix of VOCs, ...
- Validate the CFD model, in side-by-side test rooms

Publications

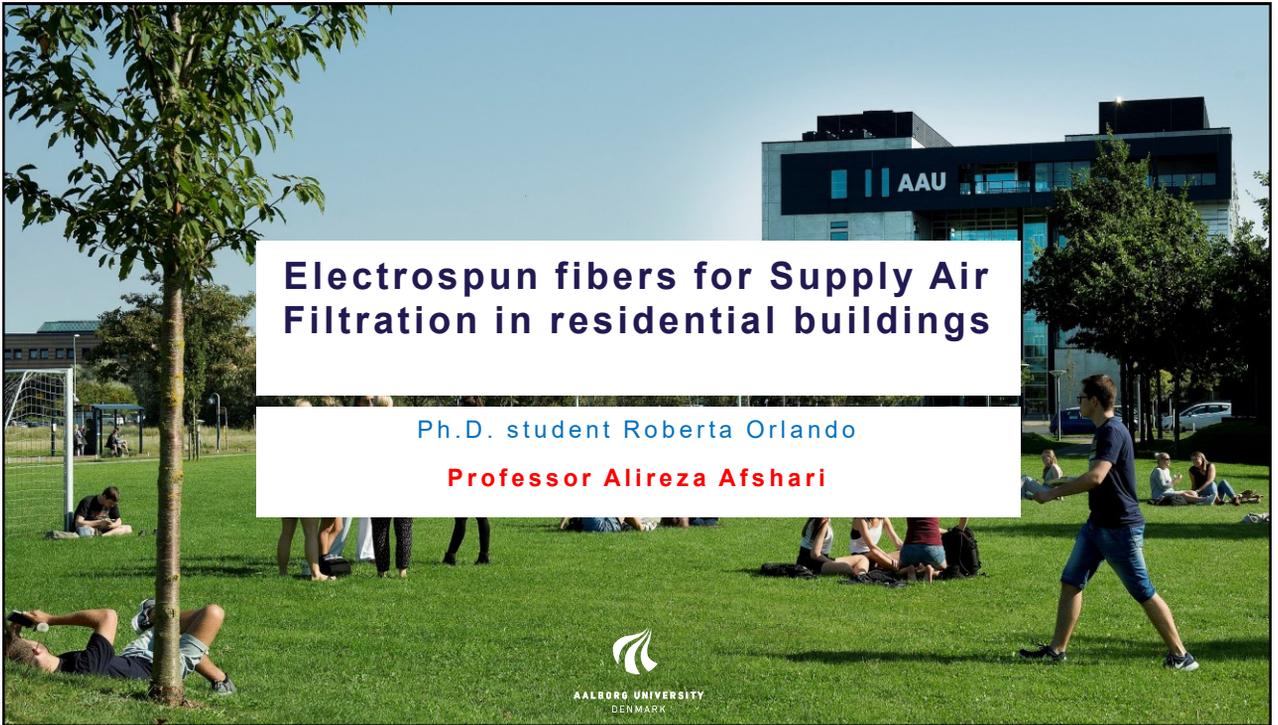
- [1] Won et al. (2021) "Development of formaldehyde flux sampler using a commercial DNPH cartridge", Building and Environment, 196, 107795.
- [2] Bahri et al. (2019) "Removal performance of formaldehyde by ceiling tiles as sorptive passive panels", Building and Environment, 160, 106172.
- [3] Zuraimi et al. (2018) "Performance of sorption- and photocatalytic oxidation-based indoor passive panel technologies", Building and Environment, 135, 85-93.

THANK YOU

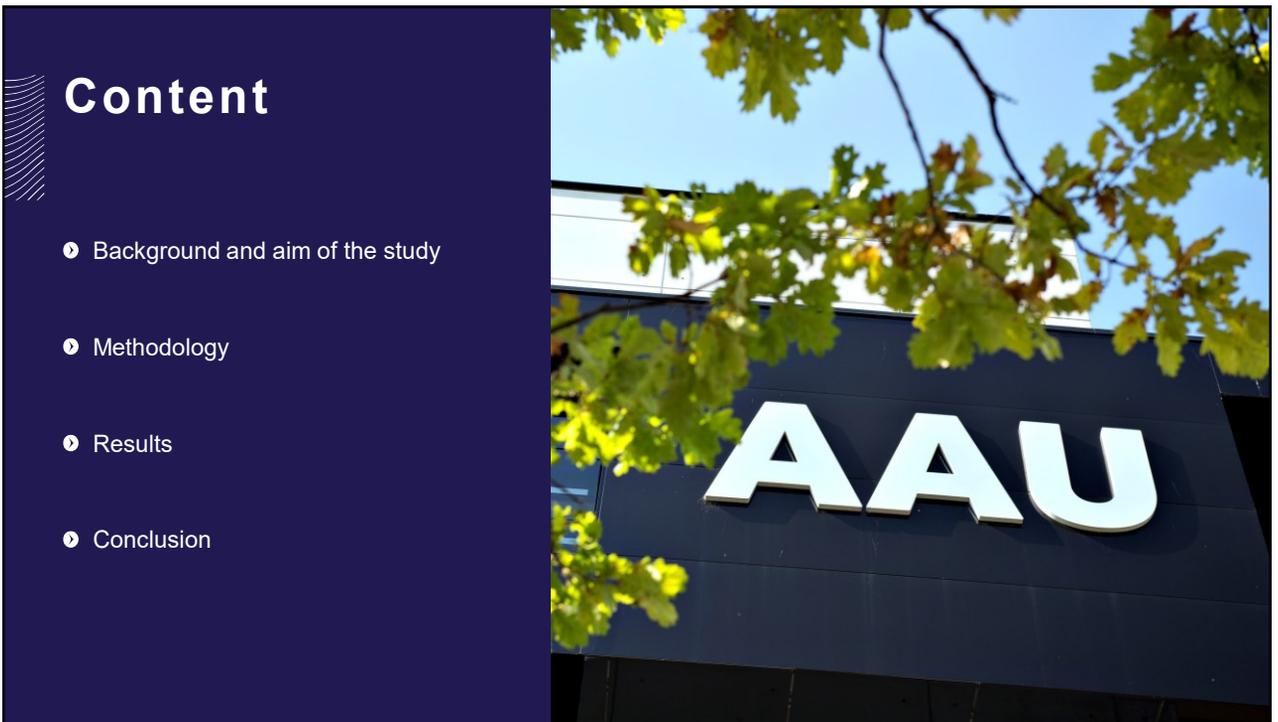
Contact Us:

Mitra Bahri : Mitra.Bahri@nrc-cnrc.gc.ca
Doyun Won: Doyun.Won@nrc-cnrc.gc.ca





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Background

3

The project's objective is to develop a **new filter material** that is able to remove both **particles and gaseous pollutants**, as part of **an air supply for residential buildings**, with the aim to improve the indoor air quality.

Indoor air quality is degraded by air pollutants of both indoor and outdoor origins. **Outdoor air pollution** can also come indoors through open windows and doors or **by supply air ventilation systems**.

The **filter's efficiency** in reducing typical indoor contaminants attributed to outdoor sources **will be evaluated under controlled conditions in the laboratory**.

The **impact of the filter** on the ventilation system's **energy use**, due to filter **pressure loss**, will be part of the investigation, as well as the assessment of the **filter quality factor**.

The **effectiveness** of the novel filter will be evaluated **under realistic condition** in naturally ventilated residential buildings.



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3

Aim of the study

The objective of the study is to develop a **novel nanofiber filter** that is effective for **both particle filtration and gaseous contaminant removal**.

The resulting filter should have a **pressure drop** that has a **minimal impact on building energy use** when **installed in the supply system**.



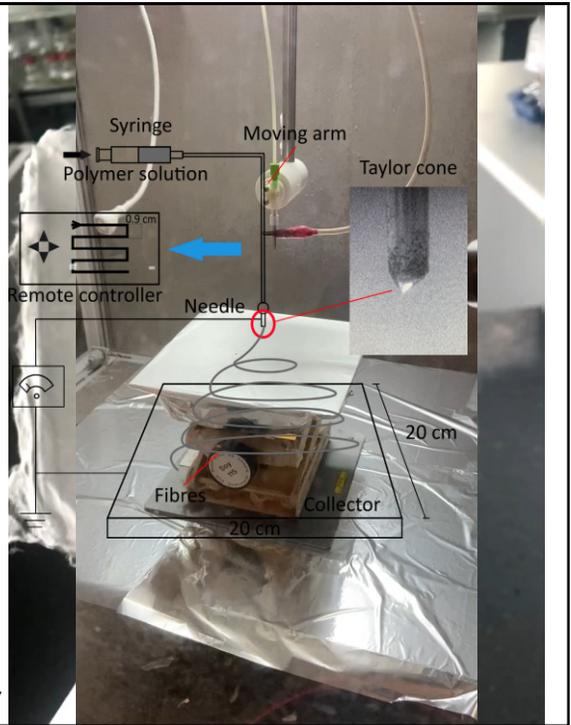
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4

Methodology

Electrospinning

- Vertical downwards in a controlled environment
- The fibers are equally distributed onto the area thanks to the movement of the needle (see video) – 10 ml solution each filter
- The result is a **porous membrane**
- Cellulose Acetate (CA)**, dissolved in acetone, is used to fabricate the fibers (polymer-based fibers from polymer/solvent solution)



5

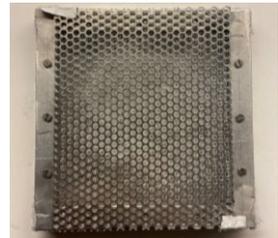
Methodology

Air spraying process

- Two solutions **sprayed separately**
 - TiO₂ nanoparticles** dispersed in a mix of 80% isopropanol and 20% ethanol
 - Activated charcoal** powder in a mix of 80% isopropanol and 20% ethanol
- Compressed air flow at 10 L/min using the **air brush** in picture. The filter lay **on the grid** positioned vertically inside a box. The solutions were sprayed **twice**:
 - 2 min spray – 1 h drying at 70 °C



Air brush



Grid



AC sprayed on the CA filter

6

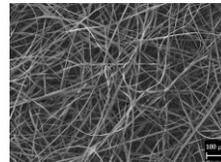
6

Methodology

Fibers characterization

- Scanning electron microscopy (SEM) images to evaluate the **fibers morphology** and the **porosity** of the filters
- The thickness of the filters was measured using an External Micrometer .

External micrometer: equipment in the image, the filters were kept between **two metal plates** to avoid compression. Accuracy ± 0.005 mm



External micrometer

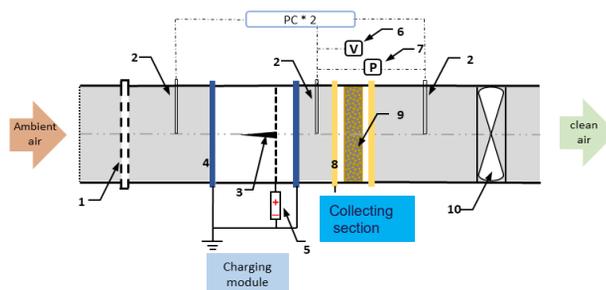


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Methodology

Air filtration performance

- The filtration module is divided into **charging section** and **collecting section**, where the membrane is kept, as visible in figure.
- Filtration efficiency of uniformly charged particles at **0.8 m/s face velocity**
- Pressure drop** in the face velocity range between **0.035 m/s to 1 m/s**



Schematic set up representation. 1. Diffusion plate, 2. Sampler, 3. Charging pins, 4. Metal rings, 5. HVDC power, 6. Anemometer, 7. Differential pressure sensor, 8. Metal mesh, 9. Membrane, 10. Fan and frequency converter

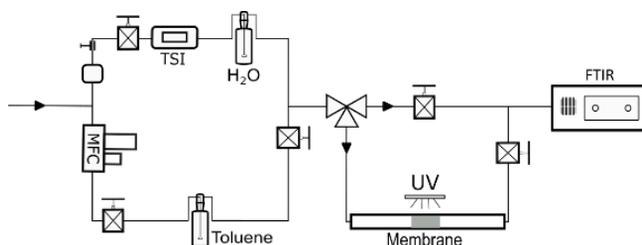


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Methodology

Air filtration performance

- Removal of gaseous compounds
 - Toluene was used
- The filters were pleated inside a quartz tube
- Blacklight blue UV lamp to initiate photocatalytic oxidation (peak wavelength at 365 nm) shined for 30 min



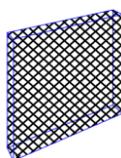
Results

Filter materials

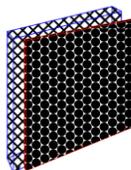
- Cellulose Acetate (CA) used in combination with two additives
 - Activated charcoal AC (adsorber)
 - Titanium dioxide TiO_2 (photocatalyst)
- Four different ultrathin filters
 1. Pure CA
 2. CA + AC
 3. CA + TiO_2
 4. Composite filter CA/AC/CA/ TiO_2



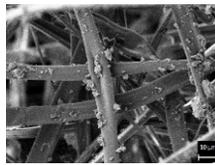
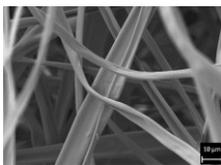
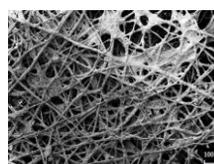
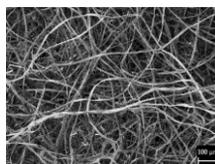
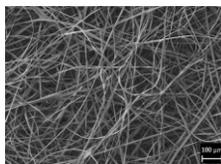
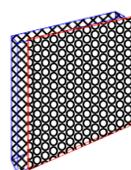
1.



2.



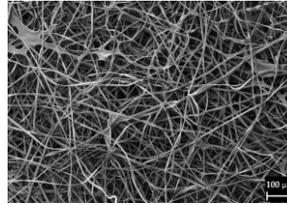
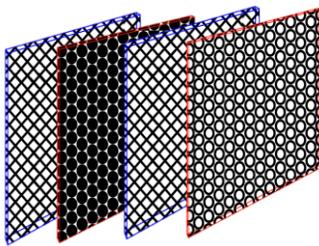
3.



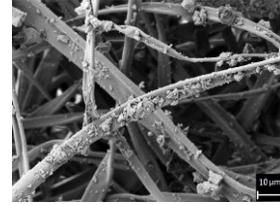
Results

Composite filter

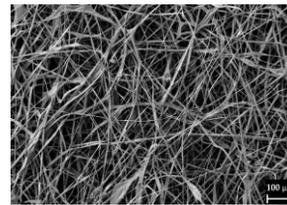
- Four layers filter
 - CA-based electrospun fibers
 - Air spraying: **Activated Charcoal**
 - CA-based electrospun fibers
 - Air spraying: **TiO₂ nanoparticles**



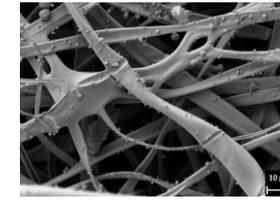
CA-based electrospun fibers



Air spraying: Activated Charcoal



CA-based electrospun fibers



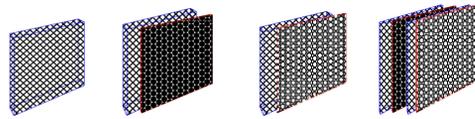
Air spraying: TiO₂ nanoparticles



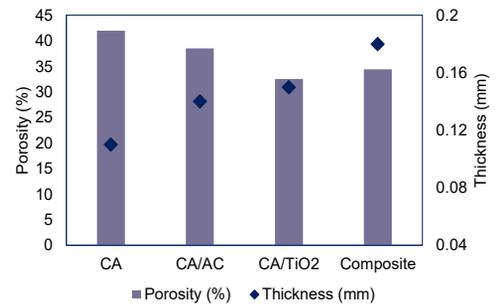
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Results

Porosity and thickness



	CA	CA/AC	CA/TiO ₂	Composite
Porosity (%)	42	38.5	32.5	34.4
Thickness (mm)	0.11	0.14	0.15	0.18



Cellulose Acetate (CA)
Activated charcoal (AC)
Titanium dioxide (TiO₂)



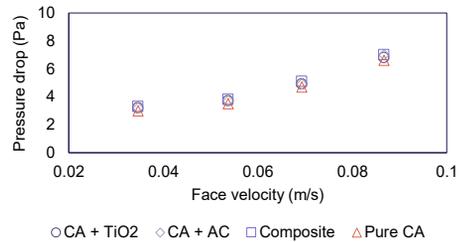
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Results

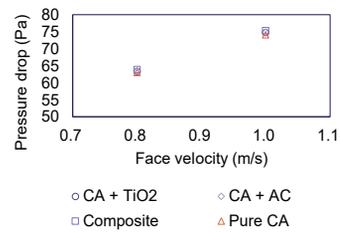
Pressure drop

- ➊ Pressure drop below 7 Pa for face velocities below 9 cm/s (natural ventilation conditions)
- ➋ The pressure drop is max 75 Pa at face velocity 1 m/s
- ➌ The use of additives increased the pressure drop.
- ➍ The composite filter recorded a non-significant increase of pressure drop compared to the pure CA filter

Pressure drop vs Face velocity
Natural ventilation



Pressure drop vs Face velocity
Mechanical ventilation



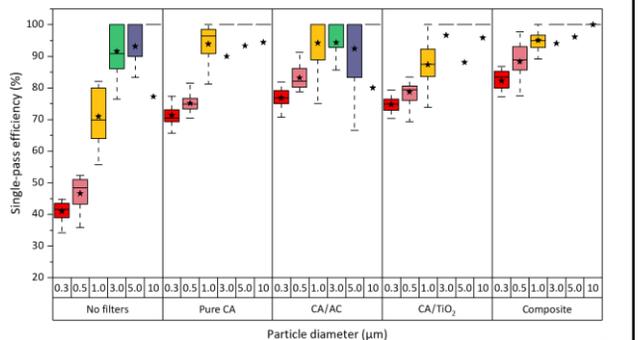
Cellulose Acetate (CA)
Activated charcoal (AC)
Titanium dioxide (TiO2)

Results

Single-pass efficiency towards uniformly charged particles

- ➊ The use of the filters has major **impact** on the filtration efficiency of small particle sizes (below 0.5 μm).
- ➋ For particle size between 0.3 μm and 0.5 μm
 - ➌ The CA/AC and CA/TiO2 filters recorded an increased filtration efficiency of 9.2% and 4.8 % respectively compared to the pure CA filter.
 - ➍ The composite filter shows improved performance compared to the other three, 16.4 % compared to the pure CA filter.
- ➎ The composite filter has a particle removal efficiency of 95% for particle size of 1 μm and 100% for particle size between 5 to 10 μm .
- ➏ High removal efficiency for particles above 3 μm size.

Single-pass efficiency (%)



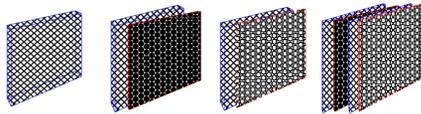
Cellulose Acetate (CA)
Activated charcoal (AC)
Titanium dioxide (TiO2)

25% ~ 75%
T Range within 1.5IQR
 Medium Line
★ Mean



Results

Quality factor: the ratio between pressure drop and filtration efficiency



	CA	CA/AC	CA/TiO ₂	Composite
Q _F (Pa ⁻¹)	0.020	0.023	0.022	0.027

Case	Particle filtration efficiency (0.3-0.5 μm) (%)	Pressure drop (Pa)	Quality factor (Pa ⁻¹)	Material	Reference
1	98	1997	0.0019	Poly(vinyl alcohol)/ Poly(acrylic acid) + silica and silver nanoparticles	[1]
2	99.98	243	0.0351	Polyimide nanofibers	[2]
3	99.992	1781	0.0053	Polysulfone/Polyacrylonitrile / Polyamide 6	[3]
4	99.997	725	0.0143	Polysulfone/TiO ₂ fibrous membrane	[4]
5	99.99	4315	0.0021	Nylon 6 nanofiber	[5]
6	99.989	659	0.0138	Polyacrylonitrile/silica nanoparticles	[6]
7	82.3	63.8	0.0271	Composite filter CA/AC/CA/TiO ₂	This work

The combination of activated charcoal and titanium dioxide into a **composite filter** has reached a **higher filtration efficiency** at the cost of a slightly increased pressure drop.

- [1] M. Zhu et al., J. Colloid Interface Sci., vol. 511, pp. 411–423, 2018.
- [2] R. Zhang et al., Nano Lett., vol. 16, no. 6, pp. 3642–3649, 2016.
- [3] S. Zhang, N. Tang, L. Cao, X. Yin, J. Yu, and B. Ding, ACS Appl. Mater. Interfaces, vol. 8, no. 42, pp. 29062–29072, 2016.
- [4] H. Wan et al., J. Colloid Interface Sci., vol. 417, pp. 18–26, 2014.
- [5] G. T. Kim, Y. C. Ahn, and J. K. Lee, Korean J. Chem. Eng., vol. 25, no. 2, pp. 368–372, 2008.
- [6] N. Wang et al., Sep. Purif. Technol., vol. 126, pp. 44–51, 2014.

Cellulose Acetate (CA)
Activated charcoal (AC)
Titanium dioxide (TiO₂)



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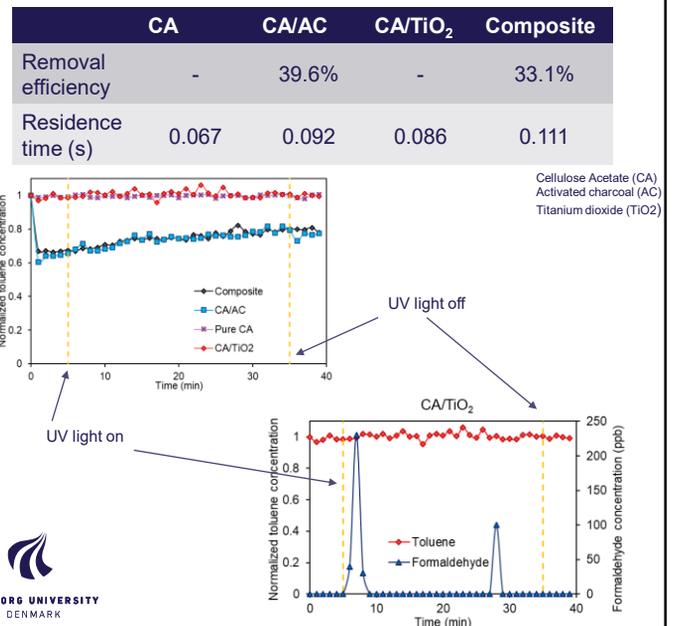
15

Results

Removal of gaseous compounds

- Toluene concentration before the filter: 22.5 ppm
- Activated charcoal does not reach the breakthrough in 40 min of testing
- The filters containing TiO₂ have shown a non-significant reduction of Toluene concentration with photocatalytic oxidation.
 - Formaldehyde production
 - Factors: related to residence time and UV intensity

The **activated charcoal** present in **CA/AC** and **composite filter** has adsorbed toluene and reached an initial removal efficiency of **39.6%** and **33.1%**.



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16

Conclusion

Summary and future work

17

- Additives have an effect on fiber morphology (porosity and surface roughness), leading to increased filtration efficiency and slightly higher pressure drop.
 - Relatively low pressure drop was achieved for all filters. Less than 7 Pa for face velocities below 9 cm/s (comparable to natural ventilation conditions).
 - Particle removal efficiency above 80% for the composite filter for particle sizes between 0.3 μm and 10 μm.
 - Activated charcoal in filter (CA+AC) and composite filter removed up to 39.6% of toluene at steady-state concentration, 22.5 ppm.
- ❑ Further investigation within the gas removal capacity especially with photocatalytic oxidation
 - ❑ UV lamp characteristics?
 - ❑ Regeneration capacity of materials
 - ❑ More experiments on simultaneous removal of a mixed particles and gaseous compound. Do they affect each other?
 - ❑ Realistic condition within a residential building. Monitoring long term performance. What is the life time of such filters?



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Cellulose Acetate (CA)
Activated charcoal (AC)
Titanium dioxide (TiO₂)

17

Thank you for your attention

18



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18

Impact of VOC and moisture buffering capacities of bio-based building materials on IAQ and indoor RH: the case of hemp concrete

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IEA Annex 86 Webinars- Smart materials- 12 Oct. 2021

1

Goal for building design

Hygrothermal comfort
Indoor air quality (IAQ)
Acoustical and visual comforts

One passive way by using hygroscopic materials (release or adsorb water vapor depending on the surrounding air conditions)

Use of vegetable particles (hemp shives, flax shives, straw bales, etc.) as building material aggregates:

- *bio-based materials*
- *low embodied energy*



Tran Le A D

2



Rape (rapeseed)



Hemp

Hemp
availability in the world

France is the first
producer of hemp
in Europe



Flax

National availability (France)



Miscanthus



Bamboo

A. D Tran Le

3

THE USES OF HEMP

STALK

TEXTILES

Lorem ipsum dolor sit amet, consectetur adipiscing elit.

INSULATION

Lorem ipsum dolor sit amet, consectetur adipiscing elit.

PAPER

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ROOTS

MEDICINE

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COMPOST

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SEED

ONLY PRODUCTS

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SEED CASE

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HEMP NUTS

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LEAVES

ANIMAL BEDDING

Lorem ipsum dolor sit amet, consectetur adipiscing elit.

PHARMA

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@Licence Freepik

Back to history



@Hemp Edification, 2015

Hemp mortar discovered in Merovingian bridge **built in the 6th century** in Saint Ceneri le Gérei, in France

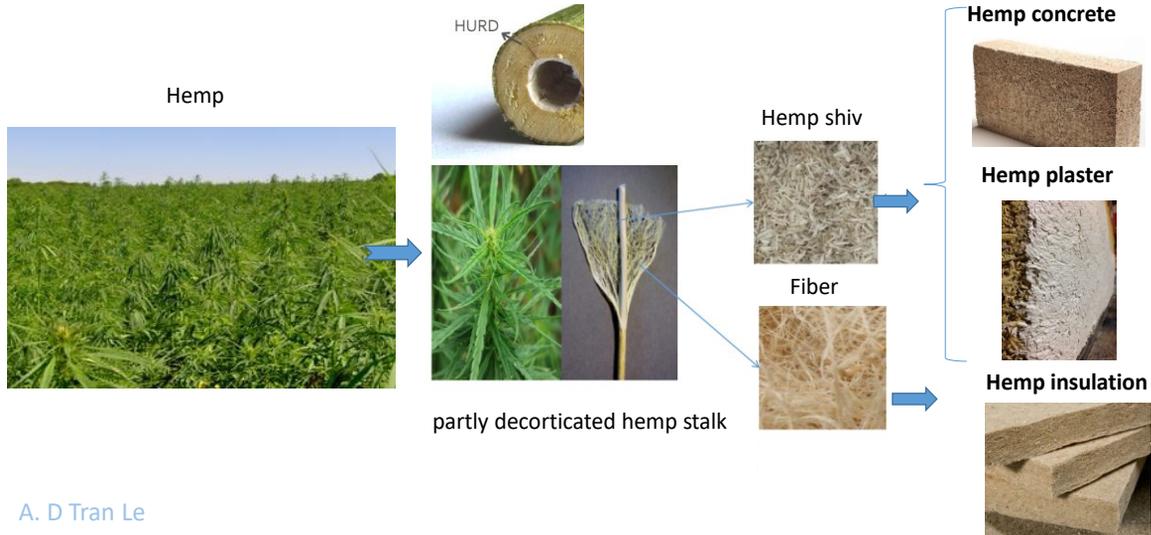
Now: hemp concrete

- ✓ environmentally friendly building material
- ✓ reference bio-based material

A. D Tran Le

4

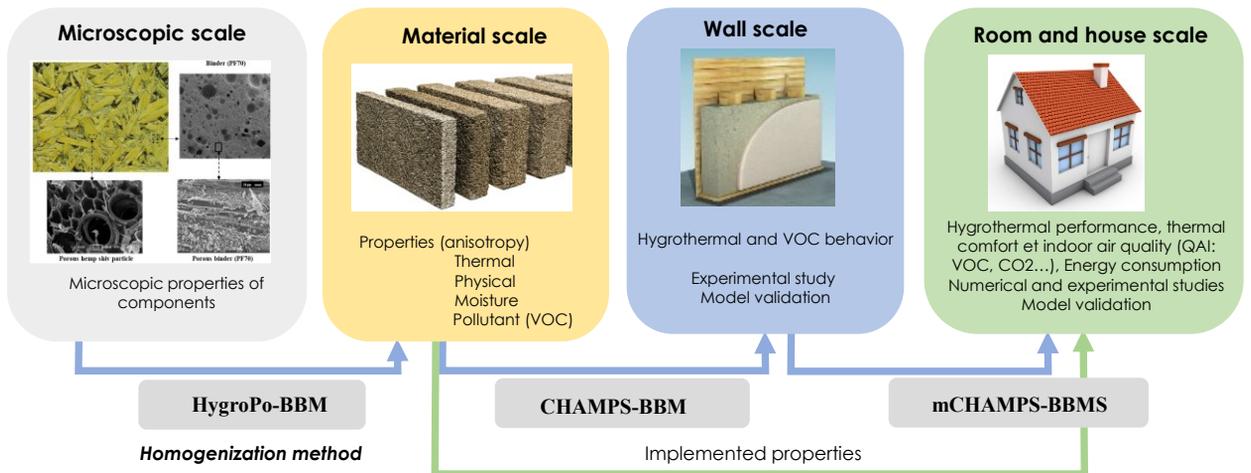
Valorization of Hemp in building construction



5

mCHAMPS-BBMS

The multi-scale approach to Coupled Heat, Air, Moisture and Pollutants Simulations in Bio-based Building Materials and Systems



Contact: Dr A.D TRAN LE, anh.dung.tran.le@u-picardie.fr

English version

6

The multi-scale approach to Coupled Heat, Air, Moisture and Pollutants Simulations in Bio-based Building Materials and Systems

What is the impact of VOC and moisture buffering capacities of hemp concrete building envelope on IAQ and indoor RH?

Wall scale



Hygrothermal and VOC behavior
Experimental study
Model validation

Room and house scale



Hygrothermal performance, thermal comfort et indoor air quality (IAQ): VOC, CO2...), Energy consumption
Numerical and experimental studies
Model validation

CHAMPS-BBM

mCHAMPS-BBMS

Homogenization method

Implemented properties

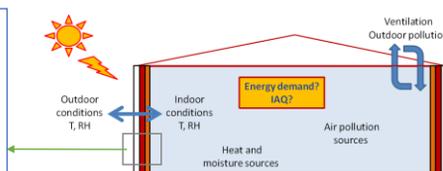
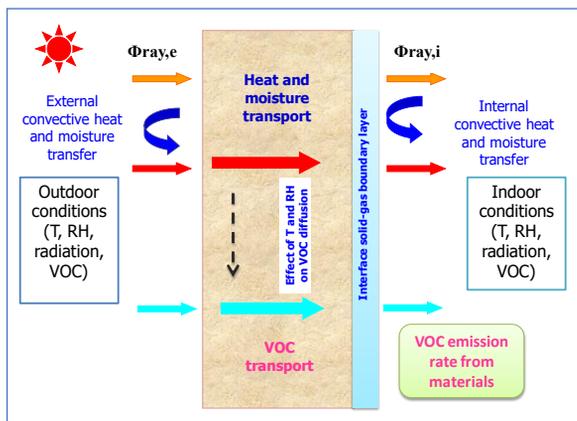
English version

A. D Tran Le

7

CHAMPS-Bio Model

Development and Validation of a Coupled Heat, Air, Moisture and Pollutant Simulation Model Dedicated to Bio-based Materials

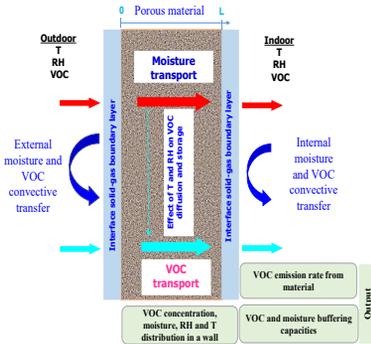


- Heat and moisture transport in building materials
- Adsorption or desorption heat due to water vapor sorption in building materials
- Diffusion and sorption of VOC
- **Taking into account of impact of T and RH on VOC diffusion and sorption (if data are available)**
- **Focusing on Biobased building materials**

A. D Tran Le

8

CHAMPS-Bio model



Selected references

- J.R. Philip, D.A. De Vries, *Moisture movement in porous materials under temperature gradients*, *Trans. Am. Geophys. Union* 38 (2) (1957) 222-232.
- J.S. Zhang, *Combined heat, air, moisture, and pollutants transport in building environmental systems*, *ISME International Journal, Series B* 48 (2) (2005) 1-9.
- N. Mendes, F.C. Winkelmann, R. Lamberts, P.C. Philipp, *Moisture effects on conduction loads*, *Energy Build.* 35 (7) (2003), 631-644.
- A.D. Tran Le, C. Maalouf, T.H. Mai, E. Wurtz, F. Collet, *Transient hygrothermal behaviour of a hemp concrete building envelope*, *Energy Build.* 42 (2010) 1797-1806.
- A.D. Tran Le, J.S. Zhang, Z. Liu, D. Samri, T. Langlet, *Modeling the similarity and the potential of toluene and moisture buffering capacities of hemp concrete on IAQ and thermal comfort*, *Building and Environment*, 188, 2021, 107455.
- etc.

Governing moisture balance equation and boundary conditions

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(D_v \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial x} \left(D_{v,e} \frac{\partial \theta}{\partial x} \right)$$

$$-\rho_l \left(D_l \frac{\partial T}{\partial x} + D_{l,e} \frac{\partial \theta}{\partial x} \right)_{x=0,e} = h_{M,e} (\rho_{ve,a,e} - \rho_{ve,s,e}) \quad \text{external surface (x=0)}$$

$$-\rho_l \left(D_l \frac{\partial T}{\partial x} + D_{l,e} \frac{\partial \theta}{\partial x} \right)_{x=L,i} = h_{M,i} (\rho_{ve,s,i} - \rho_{ve,a,i}) \quad \text{internal surface (x=L)}$$

Energy balance equation and boundary conditions

$$\rho_s C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_{app} \frac{\partial T}{\partial x} \right) + L_v \rho_l \left(\frac{\partial}{\partial x} \left(D_{v,e} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial x} \left(D_{v,e} \frac{\partial \theta}{\partial x} \right) \right)$$

$$-\lambda_{app} \frac{\partial T}{\partial x} - L_v \rho_l \left(D_{v,e} \frac{\partial T}{\partial x} + D_{v,e} \frac{\partial \theta}{\partial x} \right)_{x=0,e} = h_{T,e} (T_{a,e} - T_{s,e}) + L_v h_{M,e} (\rho_{ve,a,e} - \rho_{ve,s,e}) + \Phi_{ray,e}$$

$$-\lambda_{app} \frac{\partial T}{\partial x} - L_v \rho_l \left(D_{v,e} \frac{\partial T}{\partial x} + D_{v,e} \frac{\partial \theta}{\partial x} \right)_{x=L,i} = h_{T,i} (T_{a,i} - T_{s,i}) + L_v h_{M,i} (\rho_{ve,s,i} - \rho_{ve,a,i}) - \Phi_{ray,i}$$

Pollutants transport equation and boundary conditions

$$\frac{\partial C_m}{\partial t} = \frac{\partial}{\partial x} \left(D_m \frac{\partial C_m}{\partial x} \right)$$

$$-D_m \frac{\partial C_m}{\partial x} \Big|_{x=0,e} = h_{m,e} (C_{a,e} - C_{s,e}) \quad -D_m \frac{\partial C_m}{\partial x} \Big|_{x=L,i} = h_{m,i} (C_{s,i} - C_{a,i})$$

For pollutants model, at the material-air interface, we assume an instantaneous equilibrium between VOC concentration (mg/m3) in the air near material surface (Cas) and the one in the surface layer (Cms)

$$C_{ms} = K \cdot C_{as}$$

Energy and mass balance equations for room air

$$\rho_l C_p V \frac{\partial T}{\partial t} = \Phi_{Heat} - \Phi_{East} + \Phi_{South} - \Phi_{North} + \Phi_{Bottom} - \Phi_{Top} + \Phi_{Ventilation} + \Phi_{Source}$$

$$V \frac{\partial \rho_l}{\partial t} = Q_{InFlow} - Q_{OutFlow} + Q_{InSouth} - Q_{InNorth} + Q_{InBottom} - Q_{InTop} + Q_{InVentilation} + Q_{InSource}$$

$$V \frac{\partial C_a}{\partial t} = Q(C_{a,e} - C_{a,i}) + AE + G_{VOC_Source} \quad \text{Where} \quad E = h_{m,i} (C_{as,i} - C_{a,i})$$

The Simulation Problem Analysis and Research Kernel (SPARK)*

*SPARK: E.F. Sowell, P. Haves, *Efficient solution strategies for building energy system simulation*, *Energy Build.* 33 (2001) 309-317.



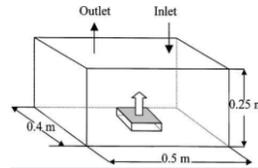
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CHAMPS-Bio model validation (1)

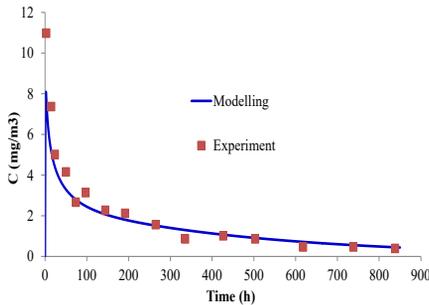
Case of a particleboard: prediction of VOC emission rate

- Experimental setup consists of a small test chamber (0.4*0.5*0.25 m3) with a pollutant emitting panel material inside
- Particleboard with dimension 0.212x0.212x0.0159 m3
- Test conditions: T=23 °C, RH=50%, Air change rate= 1 1/h

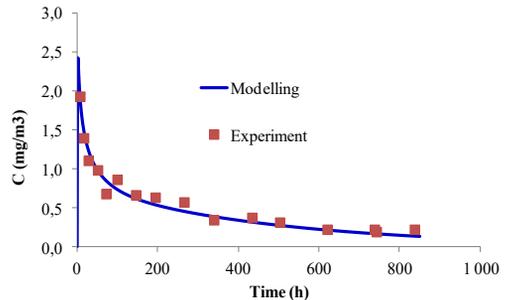
Age: 0



Reference: X. Yang, Q. Chen, J.S. Zhang, R. Magee, J. Zeng, C.Y. Shaw, *Numerical simulation of VOC emissions from dry materials*, *Build. Environ.* 36 (10) (2001) 1099-1107.



Validating for TVOC concentration emitted from the particleboard

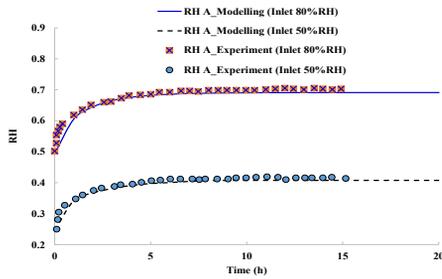


Validating for Hexanal concentration emitted from the particleboard

CHAMPS-Bio model validation (2)

CHAMPS-Bio model has been validated recently

- ✓ In framework of Fulbright Scholar program in 2020 (Commission Fulbright Franco-Américaine and Hauts-de-France region,FR)
- ✓ In collaboration with BEESL lab, Syracuse University, USA (referent Pr. ZHANG Jensen)
- ✓ Model validation with two indoor typical VOCs (*Formaldehyde and Toluene*) based on experimental results obtained with calcium silicate (Xu and Zhang 2011*)

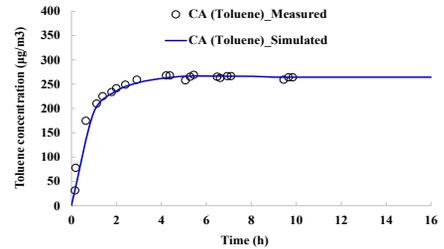


Model validation for moisture diffusion model

A.D. Tran Le, JS. Zhang, Z. Liu, D Samri, T. Langlet. Modeling the similarity and the potential of toluene and moisture buffering capacities of hemp concrete on IAQ and thermal comfort, *Building and Environment*, 188,2021,107455.

A.D. Tran Le, JS. Zhang, Z. Liu. Impact of humidity on formaldehyde and moisture buffering capacity of porous building material, *Journal of Building Engineering*, 36, 2021, 102114, ISSN 2352 7102.

Impact of humidity on VOC behavior of porous materials and on IAQ : important to study



Model validation for Toluene (TOL)

*Xu, J., Zhang, JS. An experimental study of relative humidity effect on VOCs' effective diffusion coefficient and partition coefficient in a porous medium. *Build Environ* 46 (2011), 1785-96.

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11

Effect of toluene and moisture buffering capacities of hemp concrete wall on indoor relative humidity and toluene concentration

Hemp concrete

well known in the literature

- ✓ used widely in the world
- ✓ low environmental impact
- ✓ good compromise between insulation and thermal inertia
- ✓ **high moisture buffering capacity**

Similarity between VOC and moisture buffering?
If yes, what is the impact of pollutant (VOC) buffering capacity on IAQ?



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12

Effect of toluene and moisture buffering capacities of hemp concrete wall on indoor relative humidity and toluene concentration

- Reference room: $V=5*4*2.5 \text{ m}^3$
- Ventilation rate of 0.72 ACH (Air Changes per Hour)
- Exposed surface area $S=25 \text{ m}^2$
- A toluene source scheme : 12 hours of $1000 \mu\text{g/h}$ followed intermittently 12 hours of $0 \mu\text{g/h}$
- Room is occupied by two persons from 8.00 am to 17.00 pm (the water vapor source is 142 g/h).

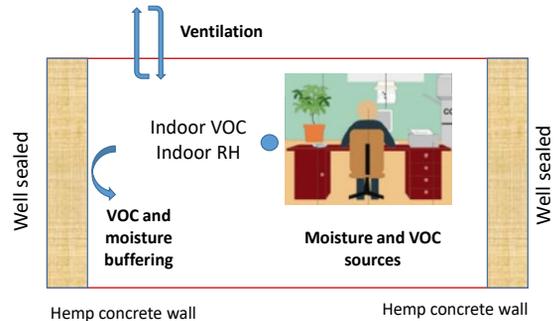
$K_{m,TOL}$	$D_{m,TOL} \text{ (m}^2/\text{s)}$
550	5.5×10^{-9}

Hygic properties of hemp concrete to model toluene properties.

Dry density (kg/m^3)	Total porosity (%)	Open porosity (%)	μ_{wv}	Sorption isotherm (GAB model parameters)
450	78	66	5	$W_m = 0.02; C_{GAB} = 7; K_{GAB} = 0.89$

Hygrothermal properties of hemp concrete measured by many research teams (selected references):

- F. Collet, J. Chamoin, S. Pretot, C. Lanos, Comparison of the hygic behaviour of three hemp concretes, *Energy Build.* 62 (2013) 294–303.
- R. Walker, S. Pavia, Moisture transfer and thermal properties of hemp–lime concretes, *Construct. Build. Mater.* 64 (2014) 270–276.
- M. Rahim, O. Douzane, A.D. Tran Le, G. Promis, B. Laidoudi, A. Crigny, et al., Characterization of flax lime and hemp lime concretes: hygic properties and moisture buffer capacity, *Energy Build.* 88 (2015) 91–99.
- T. Colinart, P. Glouannec, Temperature dependence of sorption isotherm of hygroscopic building materials. Part 1: experimental evidence and modeling, *Energy Build.* 139 (2017) 360–370.
- Etc.



- Model with buffering capacity (BC model)
- Model without buffering capacity (Without-BC model)

Toluene properties of hemp concrete

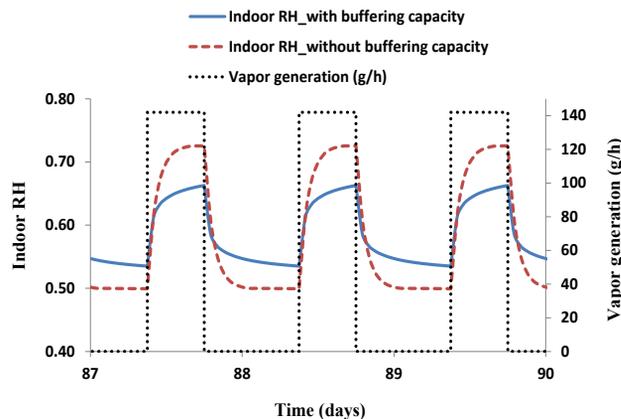
Reference: A.D. Tran Le, J.S. Zhang, Z. Liu, D Samri, T. Langlet. Modeling the similarity and the potential of toluene and moisture buffering capacities of hemp concrete on IAQ and thermal comfort, *Building and Environment*, 188,2021,107455.

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13

Effect of toluene and moisture buffering capacities of hemp concrete wall on indoor relative humidity and toluene concentration

Effect of moisture sorption capacity of hemp concrete on indoor RH



Peak reduced factor-PRF

- RH_0 : without buffering capacity Maximum values
 RH : with buffering capacity
- BC model: 66.3% RH
 - Without-BC model: 72.5% RH
 - $PRF_{RH}=8.6 \%$

$$PRF = \frac{RH_0 - RH}{RH_0}$$

Amplitude reduced factor-RFa

$$RF_a = \frac{A_0 - A}{A_0}$$

A and A_0 amplitudes of indoor relative humidity variation with and without moisture buffering capacity

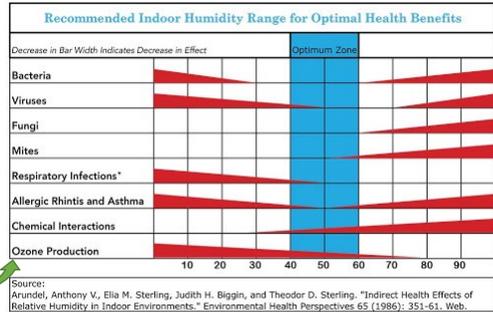
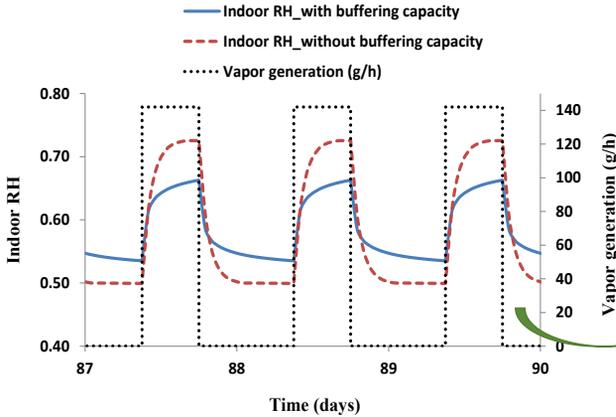
RFa value of 43.4%: moisture buffering capacity can reduce the indoor RH variation amplitude by 43.4%.

Reference: A.D. Tran Le, J.S. Zhang, Z. Liu, D Samri, T. Langlet. Modeling the similarity and the potential of toluene and moisture buffering capacities of hemp concrete on IAQ and thermal comfort, *Building and Environment*, 188,2021,107455.

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14

Discussion: Effect of moisture sorption capacity of hemp concrete on health benefits

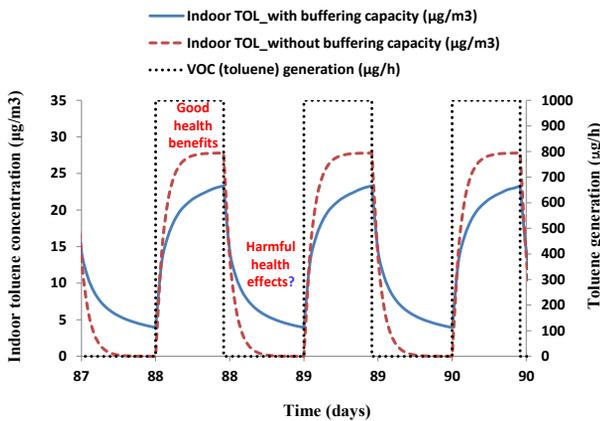


Moisture buffering capacity
passive way to keep the variation in RH between threshold levels

→ ✓ Hygrothermal comfort
✓ Health benefits

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Effect of toluene (TOL) sorption capacity of hemp concrete on indoor toluene concentration



Similarity between VOC and moisture buffering

Peak reduced factor-PRF

C_0 : without buffering capacity
 C : with buffering capacity

$$PRF = \frac{C_0 - C}{C_0}$$

Maximum values
 • BC model: 23.6 µg/m³
 • Without-BC model: 27.8 µg/m³
 $PRF_{TOL} = 15\%$

Cumulative Exposure Reduction Factor, ERFc

takes into account the concentration reduction and exposure time

$$ERF_c = \int_0^t PRF dt$$

The ERFc for toluene is 210.5% for 12 h exposure

Health benefits?

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Reference: A.D. Tran Le, J.S. Zhang, Z. Liu, D Samri, T. Langlet. Modeling the similarity and the potential of toluene and moisture buffering capacities of hemp concrete on IAQ and thermal comfort, *Building and Environment*, 188,2021,107455.

Conclusions

- ✓ Similarity between toluene (VOC) and moisture buffering capacities of hemp concrete (a reference bio-based building material)
- ✓ Impact of buffering capacities (toluene-VOC and moisture) of hemp concrete on indoor RH and IAQ: important to study
 - VOC buffering capacity: special attention at health benefits?
- Needed further experiments and analyses
- If confirmed: buffering capacity toward moisture/pollutant (VOC) as an approach to improving IAQ as well as hygrothermal performance of buildings in future standards and design



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Thank you for your attention

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