Modélisation des phénomènes de transfert de chaleur et de masse dans les matériaux poreux du bâtiment

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Transferts thermo-hydriques multi-échelles : du végétal au climat, 4 Décembre 2025

Context

Building energy consumption in the world:

- 20 % CO_2 emission,
- 33 % of the energy consumption.

Issues for the building energy efficiency:

- build and retrofit low-energy buildings,
- avoid durability problems.

For this purpose, models:

- to estimate the energy consumption,
- to understand the heat and mass behaviour of the building,
- to anticipate the disorders,
- at the end to choose the best construction options.

mold growth after bad retrofit

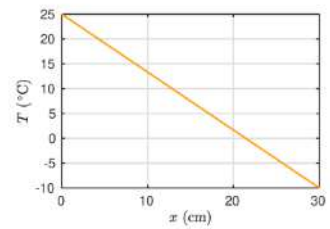
coating shrinking after bad retrofit

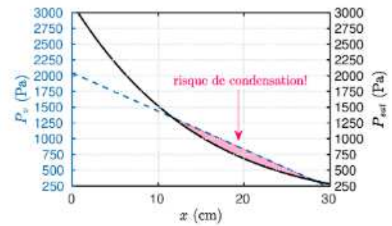
One of the first model (still used)

Condensation risk: Glaser method

- Hypothesis:
  - steady state heat and mass transfer
  - constant (scalar) properties
  - uncoupled phenomena

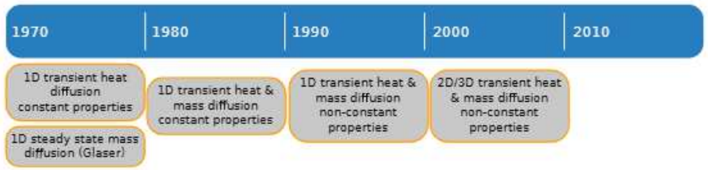
- Four steps:
  1. Plot the temperature in the wall,
  2. Plot the vapor profile in the wall,
  3. Plot the saturation pressure in the wall,
  4. Determine if there is condensation.





State-of-the-art

Several mathematical models since the 1^{st} oil crisis

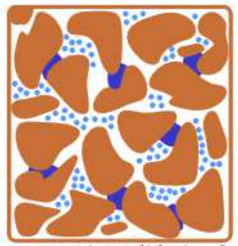


Several experimental demonstrators

- several scales: material, wall, building
- several materials: classical, bio-based, geo-based, etc.

Modeling heat and mass transfer
Important quantities

- porous material, several species:
  - solid matrix,
  - water vapor,
  - liquid water,
  - dry air.
- Porosity



$$\pi = \frac{V_{voids}}{V_{tot}}$$

with

$$V_{tot} = V_0 + V_{voids}$$

Physical phenomena

Important quantities

- temperature $T\ \left[\mathsf{K}\right]$ (assumed equal for every specie)
- mass content $i \in \left\{1, 2, 3\right\}$:
  - mass dry basis

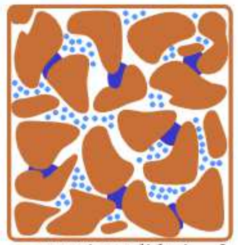
$$\theta_i = \frac{m_i}{m_0} \quad \left[\mathrm{kg\,.\,kg}^{-1}\right]$$

  - volume dry basis

$$\omega_i = \frac{V_i}{V_0} \quad \left[\mathrm{m}^3\,.\,\mathrm{m}^{-3}\right]$$

  - concentration

$$\rho_i = \frac{m_i}{V_0} \quad \left[\mathrm{kg\,.\,m}^{-3}\right]$$


matrice solide $i = 0$
eau vapeur $i = 1$
eau liquide $i = 2$
air sec $i = 3$

Mass and heat flux

- Flux
  - heat flux density j $\left[\mathrm{W\,.\,m^{-2}}\right]$
  - mass flux density g_i $\left[\mathrm{kg\,.\,s^{-1}\,.\,m^{-2}}\right]$
- Phenomenological law
  - FOURIER's law (1822):

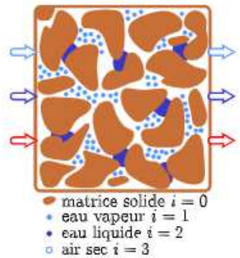
$$\boldsymbol{j} = -\lambda\,\boldsymbol{\nabla} T$$

with λ $\left[\mathrm{W\,.\,m^{-1}\,.\,K^{-1}}\right]$ material thermal conductivity

  - FICK's law (1855):

$$\boldsymbol{g}_i = -\rho_0\,D_i\,\boldsymbol{\nabla}\theta_i$$

with D_i $\left[\mathrm{m^2\,.\,s^{-1}}\right]$ diffusion coefficient of specie i



Mathematical model

Mass conservation equation

- Law:

The mass quantity of specie i in the volume V exchanged with the outside, over any time interval, includes:

- the quantity exchanged at the boundary surface S
- the quantity provided by sources in the volume: $\Sigma_i \left[\mathrm{kg} \, . \, \mathrm{m}^{-3} \, . \, \mathrm{s}^{-1} \right]$

$$\iiint_V \rho_0 \frac{\partial \theta_i}{\partial t} \, \mathrm{d}V = - \oiint_S \boldsymbol{g}_i \cdot \boldsymbol{n} \, \mathrm{d}S + \iiint_V \Sigma_i \, \mathrm{d}V$$

which provides (Gauss–Ostrogradski + Fick)

$$\frac{\partial \theta_i}{\partial t} = \nabla \cdot \left(D_i \nabla \theta_i \right) + \Sigma_i$$

Mathematical model

Mass conservation equation

- Assumptions:
  - dry air movement is negligible,
  - no chemical reactions,
  - Σ_i only related to phase change (liquid $\leftrightarrow$ vapor) $\Sigma_1 + \Sigma_2 = 0$
  - moisture content $\theta = \theta_1 + \theta_2 \approx \theta_1$
  - no thermo-diffusion.
- Final mass conservation equation

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left(D_\theta \nabla \theta \right)$$

with $D_\theta = D_1 + D_2$

- Can be formulated using other physical quantities: vapor pressure, relative humidity, capillary pressure...

Mathematical model

Mass conservation equation

What choice for potential?

- moisture content

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \Big(D_\theta \, \nabla \theta \Big)$$

- vapor pressure/relative humidity

$$\xi(\varphi)\,\frac{\partial \varphi}{\partial t} = \nabla \cdot \Big(D_\theta \, \xi(\varphi) \nabla \varphi \Big)$$

$\Rightarrow$ be aware with non-linearities

	Nonlinearity quantification	
GAB model	$\varphi \in \big[0.2\,,\,0.7\big]$	$\varphi \in \big[0.9\,,\,1.0\big]$
Material	$\mathcal{L}_2\Big(D_\theta \cdot \xi(\phi)\Big)$	$\mathcal{L}_2\Big(D_\theta \cdot \xi(\phi)\Big)$
AAC	1.01	1.5
WFI	2.27	5.49
HC	6.12	249.27

Mathematical model

Energy conservation equation

▶ 1[st] thermodynamic law: The heat exchange in the volume V with the outside, over any time interval, includes:

- the rate of heat transfer exchanged at the boundary surface S
- the rate of heating by sources in the volume: $\mathcal{P}\ \left[\mathrm{W\,.\,m^{-3}\,.\,s^{-1}}\right]$

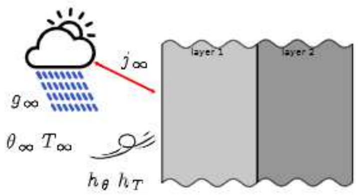
$$\iiint_V \frac{\partial h}{\partial t}\,\mathrm{d}V \;=\; -\oiint_S \boldsymbol{j}\cdot\boldsymbol{n}\,\mathrm{d}S \;-\; -\oiint_S \sum_{i=1}^{2} \frac{h_i}{\rho_0}\,\boldsymbol{g}_i\cdot\boldsymbol{n}\,\mathrm{d}S \;+\; \iiint_V \mathcal{P}\,\mathrm{d}V$$

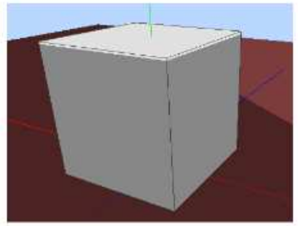
which provides (Gauss–Ostrogradski + Fick + Fourier + mass cons. eq.)

$$\left(\rho_0\,c_0 \;+\; \sum_{i=1}^{2}\rho_0\,c_i\,\theta_i\right)\frac{\partial T}{\partial t} \;=\; \boldsymbol{\nabla}\cdot\left(\lambda\,\boldsymbol{\nabla} T\right) \;+\; h_{12}\,\boldsymbol{\nabla}\cdot\left(D_1\,\boldsymbol{\nabla}\theta_1\right)$$

Mathematical model

Boundary conditions





- Heat transfer:

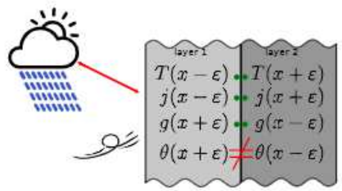
$$\lambda \nabla T \cdot \boldsymbol{n} + h_q T = \underbrace{h_T T_\infty}_{\text{convection}} + \underbrace{j_\infty}_{\text{radiation (SW + LW)}}$$

- Mass transfer:

$$D_\theta \nabla\theta \cdot \boldsymbol{n} + h_\theta \theta = \underbrace{h_\theta \theta_\infty}_{\text{convection}} + \underbrace{g_\infty}_{\text{rain, rising damps, etc.}}$$

Mathematical model

interface conditions



- Heat transfer:

$$\left(\lambda \nabla T\right)\Big|_{x-\varepsilon} \cdot \boldsymbol{n} = -\left(\lambda \nabla T\right)\Big|_{x+\varepsilon} \cdot \boldsymbol{n}$$

$$T\Big|_{x-\varepsilon} = T\Big|_{x+\varepsilon}$$

- Mass transfer:

$$\left(D_\theta \nabla \theta\right)\Big|_{x-\varepsilon} \cdot \boldsymbol{n} = -\left(D_\theta \nabla \theta\right)\Big|_{x+\varepsilon} \cdot \boldsymbol{n}$$

$$\theta\Big|_{x-\varepsilon} \neq \theta\Big|_{x+\varepsilon} \Rightarrow P_i\Big|_{x-\varepsilon} = P_i\Big|_{x\varepsilon}$$

Mathematical model

A system of two coupled ordinary differential equations:

$$
\begin{aligned}
c_m^{\star} \frac{\partial u}{\partial t} &= \mathrm{Fo}^{\,\mathrm{m}} \, \boldsymbol{\nabla} \cdot \left(k_m^{\star} \, \boldsymbol{\nabla} u \right), \\
c_q^{\star} \frac{\partial v}{\partial t} &= \mathrm{Fo}^{\,\mathrm{q}} \, \boldsymbol{\nabla} \cdot \left(k_q^{\star} \, \boldsymbol{\nabla} v \right) + \mathrm{Fo}^{\,\mathrm{qm}} \, \boldsymbol{\nabla} \cdot \left(k_{qm}^{\star} \, \boldsymbol{\nabla} u \right).
\end{aligned}
$$

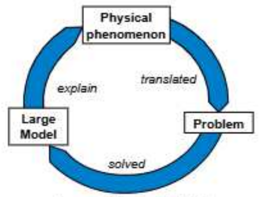
Where are the challenges of this mathematical problem?

1. the time scales of the problem,
2. the non-linear coefficients,
3. the spatial geometries,
4. the boundary conditions.

Numerical models for HM transfer

Large original model (LOM):

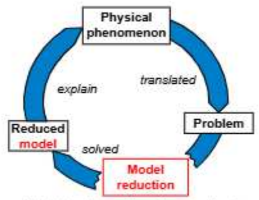
- solution $u(x, t)$,
- degree of freedom of the solution: $N = N_x \times N_t$.



Large Original Model

Reduced Order model (ROM):

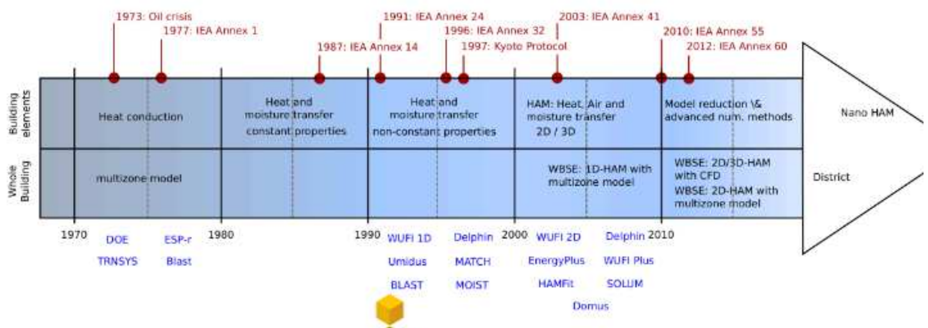
- the fidelity of the physical model is not reduced,
- solution $\tilde{u}(x, t)$,
- degree of freedom of the solution: $N \ll N_x \times N_t$.



Model order reduction methods

Existing software for modeling

non-exhaustive list [1, 2]



Determining material transfer properties

- several important properties:
  - vapor permeability
  - sorption curve
  - thermal conductivity
  - specific heat capacity
  - porosity
  - Moisture Buffer Value (MBV)

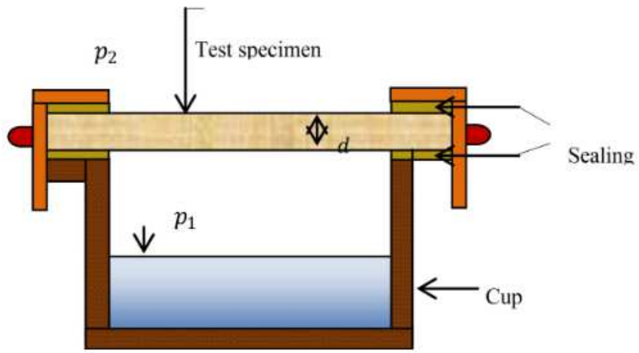
(vapor permeability, sorption curve, thermal conductivity, specific heat capacity): required for modeling

(Moisture Buffer Value): engineering purposes

Determining material transfer properties

vapor permeability

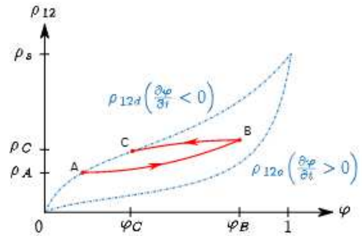
- cup method (EN ISO 12572)
  - samples of diameter ~ 8 cm, thickness max 5.5 cm
  - steady state measurement
  - saturated salts

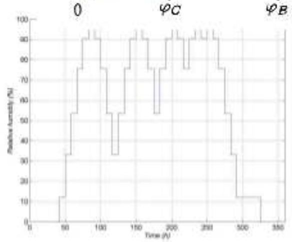


Determining material transfer properties

sorption curve

- ▶ Dynamic Vapor Sorption (DVS)
  - smashed samples ∼ 100 mg
  - initial condition: dry state
  - investigation of hysteresis





Determining material transfer properties

sorption curve

Several models [3]:

Brunauer, Emmett and Teller (BET) model:

$$u\left(p_1, p_2, \varphi\right) = \frac{p_1\, p_2}{\left(1 - \varphi\right)\left(1 + \left(p_2 - 1\right)\varphi\right)} \cdot \varphi$$

Guggenheim–Anderson–de Boer (GAB) model:

$$u\left(p_1, p_2, p_3, \varphi\right) = \frac{p_1\, p_2\, p_3}{\left(1 - p_2\,\varphi\right)\left(1 - p_2\,\varphi + p_2\, p_3\,\varphi\right)}\, \varphi$$

Oswin model: $u\left(p_1, p_2, \varphi\right) = p_1 \cdot \left(\frac{\varphi}{1 - \varphi}\right)^{p_2}$

van Genuchten model:

$$u\left(p_1, p_2, p_3, \varphi\right) = p_1 \cdot \left(1 + \left(p_2\, P_2(\varphi)\right)^{p_3}\right)^{-1 + \frac{1}{p_3}}$$

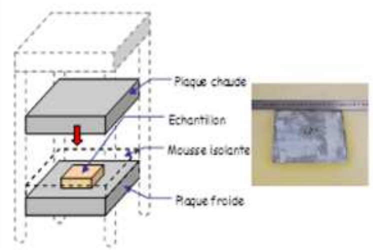
MADS model:

$$u\left(p_1, p_2, \varphi\right) = \frac{K}{p_2 \cdot \left(1 + \tan(p_1)^2\right)} \cdot \left(\tan(p_1 + p_2\,\varphi) - \tan(p_1)\right)$$

Determining material transfer properties

thermal conductivity

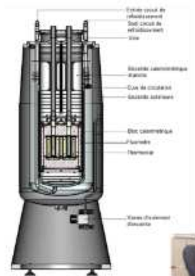
- Guarded hot plate
  - samples from 15 × 12 cm^2 to 50 × 50 cm^2
  - steady state measurement
  - around 24 h for 3 temperature range



Determining material transfer properties

specific heat capacity

- DSC
  - samples $\sim$ 10 mg
  - 2D heat flux
  - around 10 min



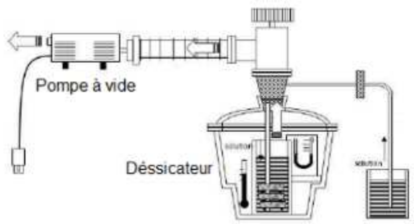
- Calvet Calorimeter
  - samples $\sim$ 1 cm diameter, $\sim$ 5 cm thickness,
  - 3D heat flux
  - around 24 h

Dispositif expérimental de mesure de la chaleur spécifique « DSC Q100 »

Determining material transfer properties

porosity

- accessible by water



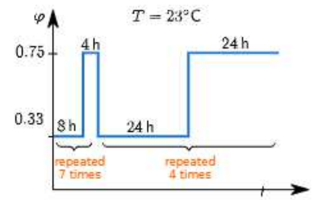
- accessible by mercury

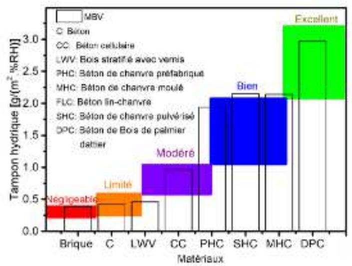
Determining material transfer properties

moisture buffer value

- Nordtest protocol
- cyclic solicitations in climatic chamber
- around 12 days

$$MBV = \frac{m_{\max} - m_{\min}}{A\left(\varphi_{\max} - \varphi_{\min}\right)}$$





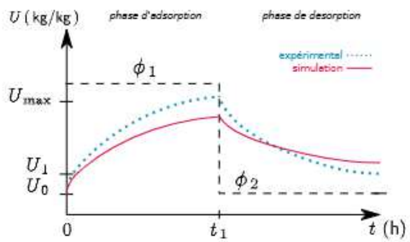
Conclusion

Synthesis

- a system of coupled partial differential equations,
- commercial software or home made codes,
- several properties to determine based on standard methods.

However,

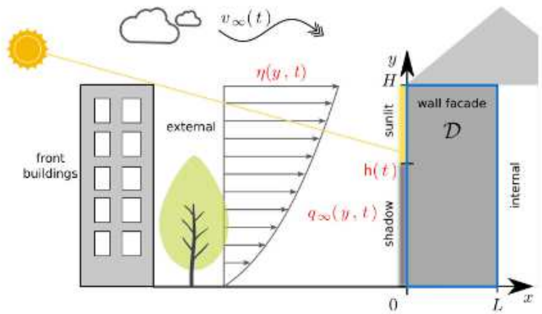
- ▶ Long-term observations?
- ▶ Some discrepancies observed [4]:
  - for different materials,
  - for different facilities,
  - at different scales: material & wall.

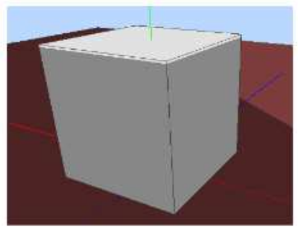


Open-challenges

Improving the reliability of heat and mass transfer models:

- scaled experimental models for long-term analyses,
- advanced modelling:
  - (a) hysteresis effects on the water sorption;
  - (b) effect of air transfer on heat and water mass;
  - (c) consideration of the spatial variations of the boundary conditions.





Thank you for your attention

Some references I

[1] N. Mendes, M. Chhay, J. Berger, and D. Dutykh. *Numerical Methods for Diffusion Phenomena in Building Physics: A Practical Introduction*. Springer International Publishing, 2019.

[2] M. Woloszyn and C; Rode. Tools for performance simulation of heat, air and moisture conditions of whole buildings. *Building Simulation*, 1(1):5–24, 2008.

[3] J. Berger, T. Colinart, B.R. Loiola, and H.R.B. Orlande. Parameter estimation and model selection for water sorption in a wood fibre material. *Wood Science and Technology*, 54(6):1423–1446, 2020.

[4] T. Busser, J. Berger, A. Piot, M. Pailha, and M. Woloszyn. Comparison of model numerical predictions of heat and moisture transfer in porous media with experimental observations at material and wall scales: An analysis of recent trends. *Drying Technology*, 37(11):1363–1395, 2019.