Situations de non-équilibre local durant les transferts couplés chaleur/humidité dans les matériaux de construction biosourcés.

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CentraleSupélec

LGPM
GÉNIE DES PROCÉDÉS ET MATÉRIAUX

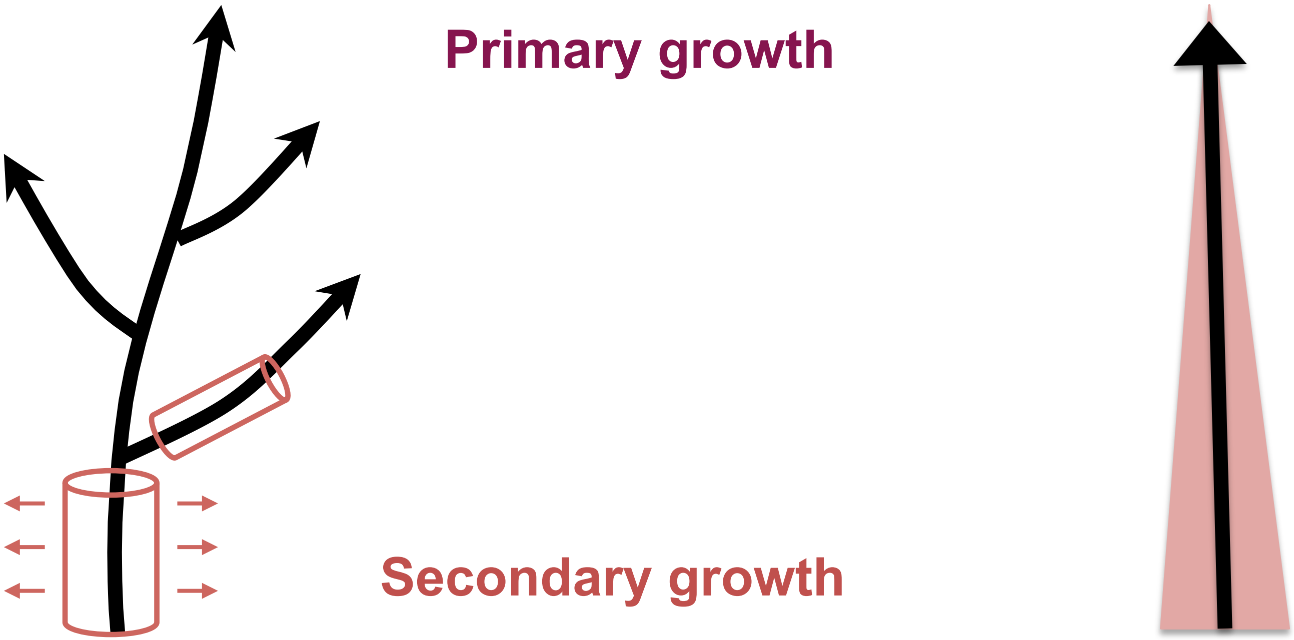
Vos 20 prochaines minutes

- Généralités sur les matériaux bio-sourcés
- Formulation macroscopique des transferts couplés
- Phénomènes locaux responsable du non-équilibre local
- Quelques résultats de modélisation à double échelle de porosité
- Conclusions et perspectives

Matériaux bio-sourcés = tiges des plantes

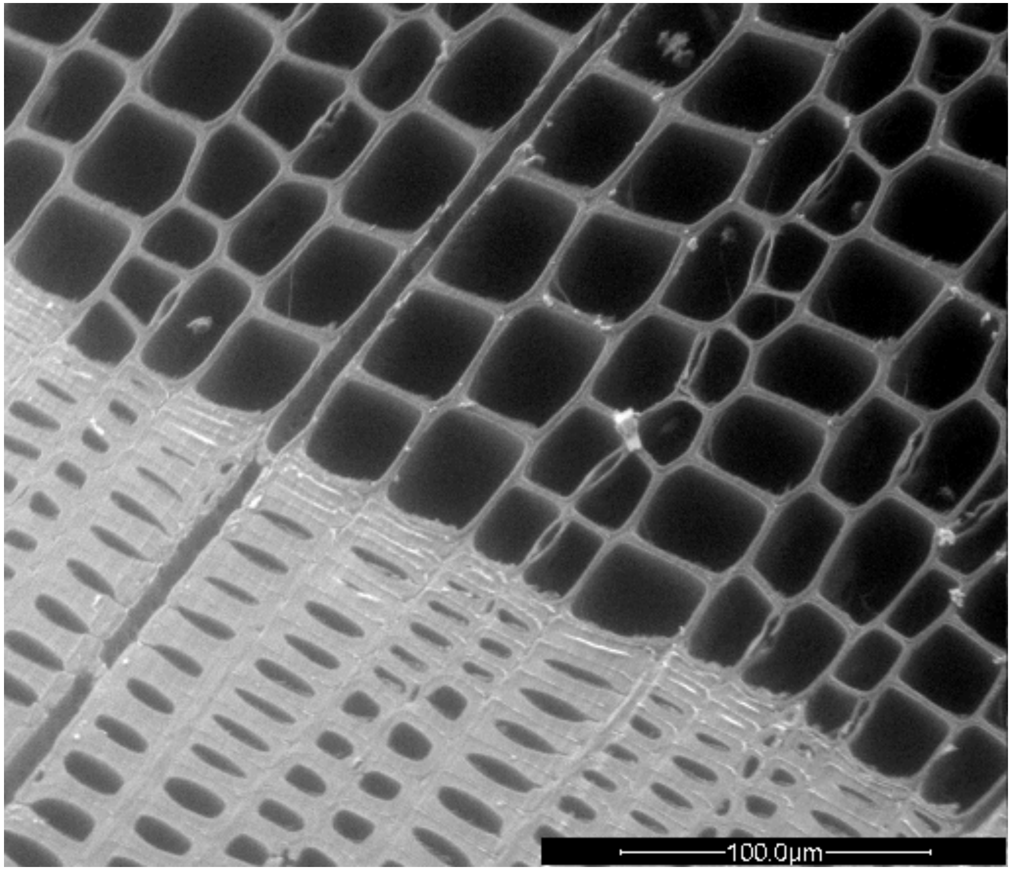
Major roles of stems in plants

- ***Vascular system***
- ***Mechanical support***
- ***Shape adaptation***
- ***Resistance to biological attacks***

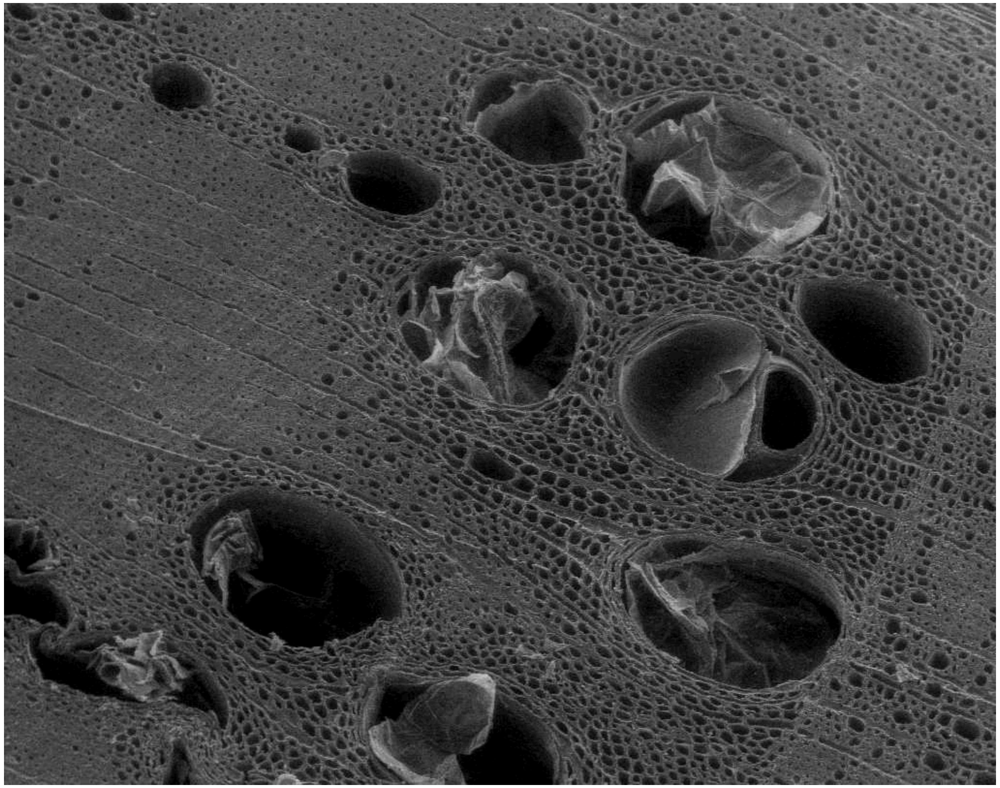


Trees

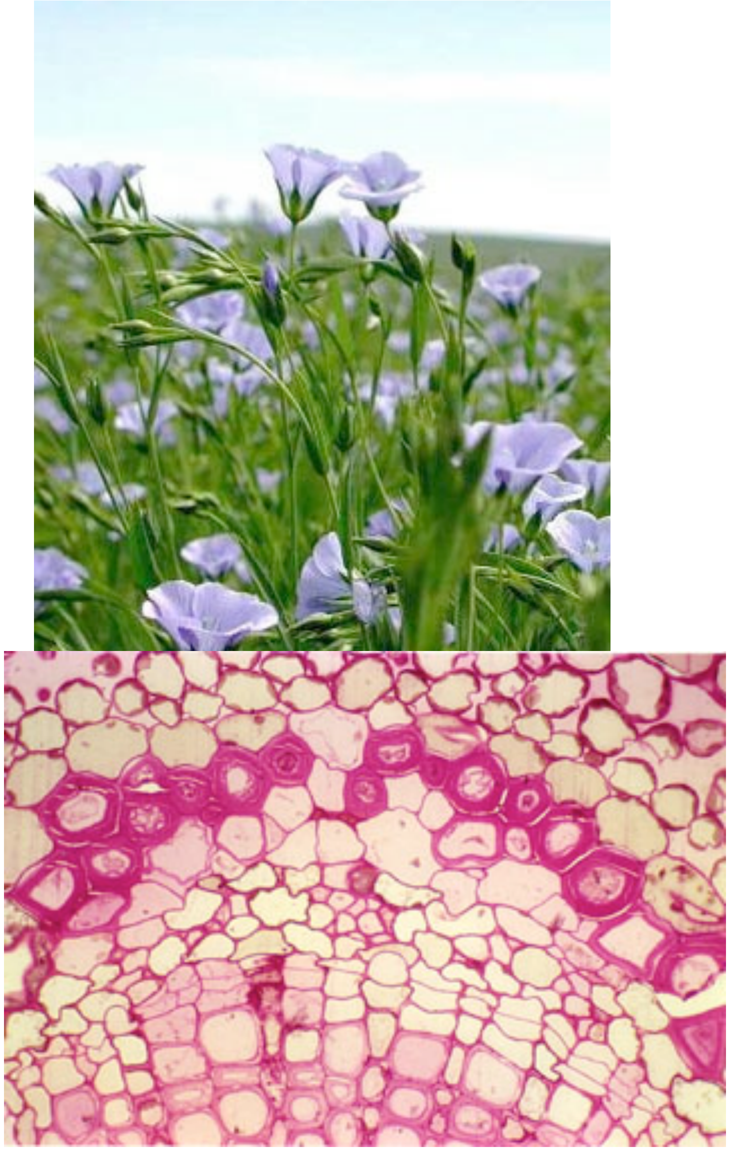
Annual plants



ESEM image of Spruce, P. Perré



ESEM image of Oak, P. Perré



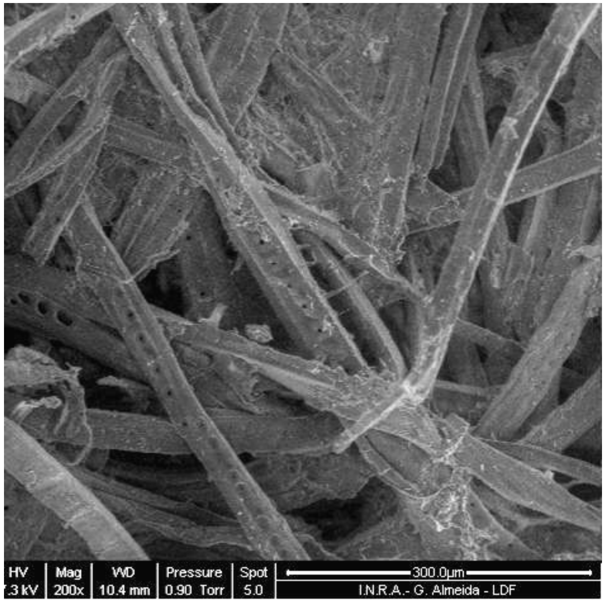
Lin (*Linum usitatissimum* L.)

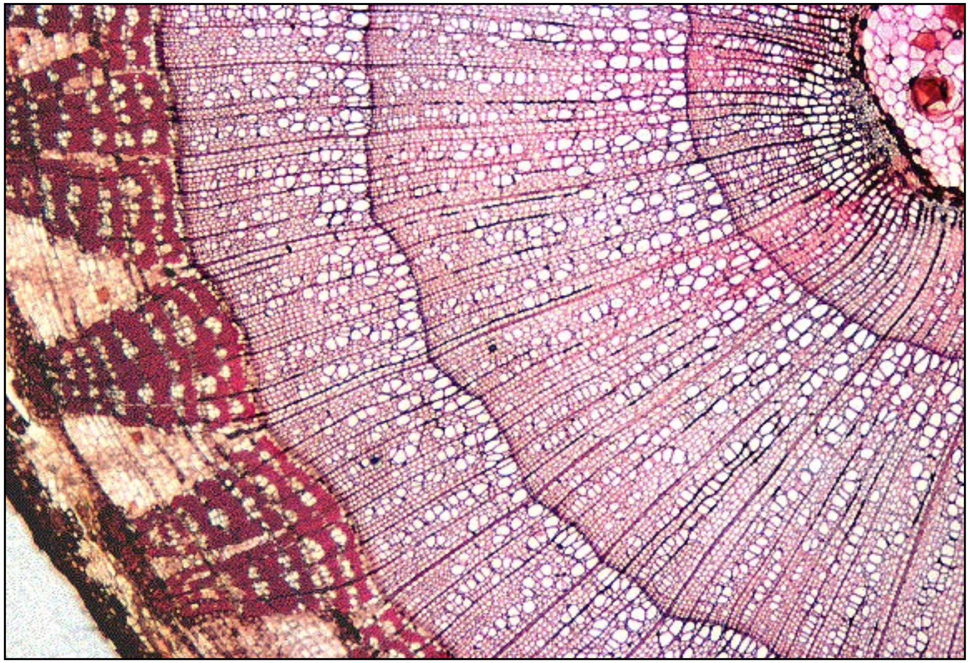
Chanvre (*Cannabis sativa*)

Sources : [*http://www.snv.jussieu.fr/bmedia/textiles*](http://www.snv.jussieu.fr/bmedia/textiles)
http://www.chanvre.com/

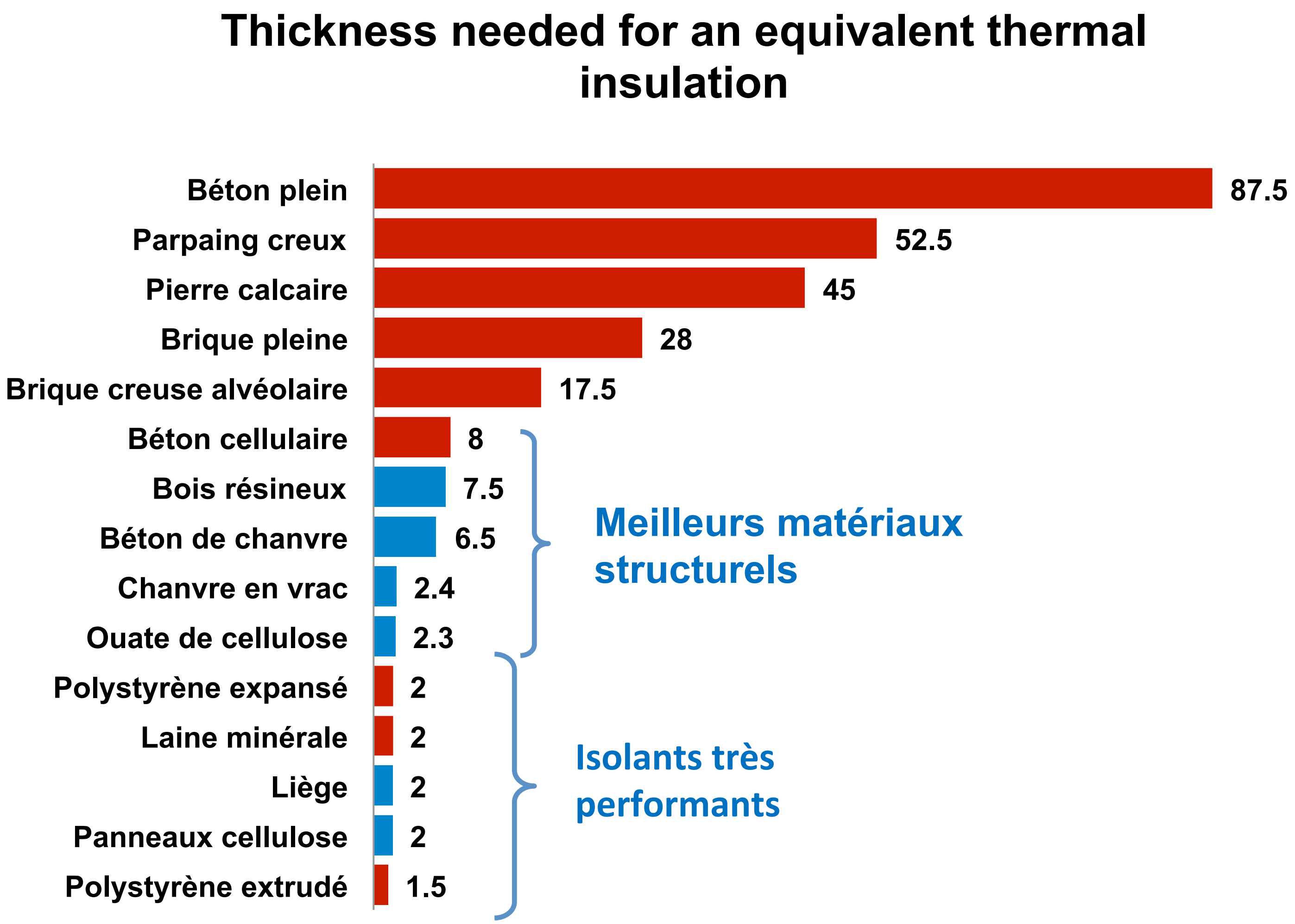
Intérêt des matériaux bio-sourcés

- Fibres végétales = matériau très élaboré
- Combinaison unique de propriétés
    - Rigide et résilient en traction et compression
    - Faible conductivité thermique (le top des matériaux structurels)
- Peu d'énergie nécessaire à la transformation
- Stockage du CO_2 fixé par photosynthèse
- De nombreux composites

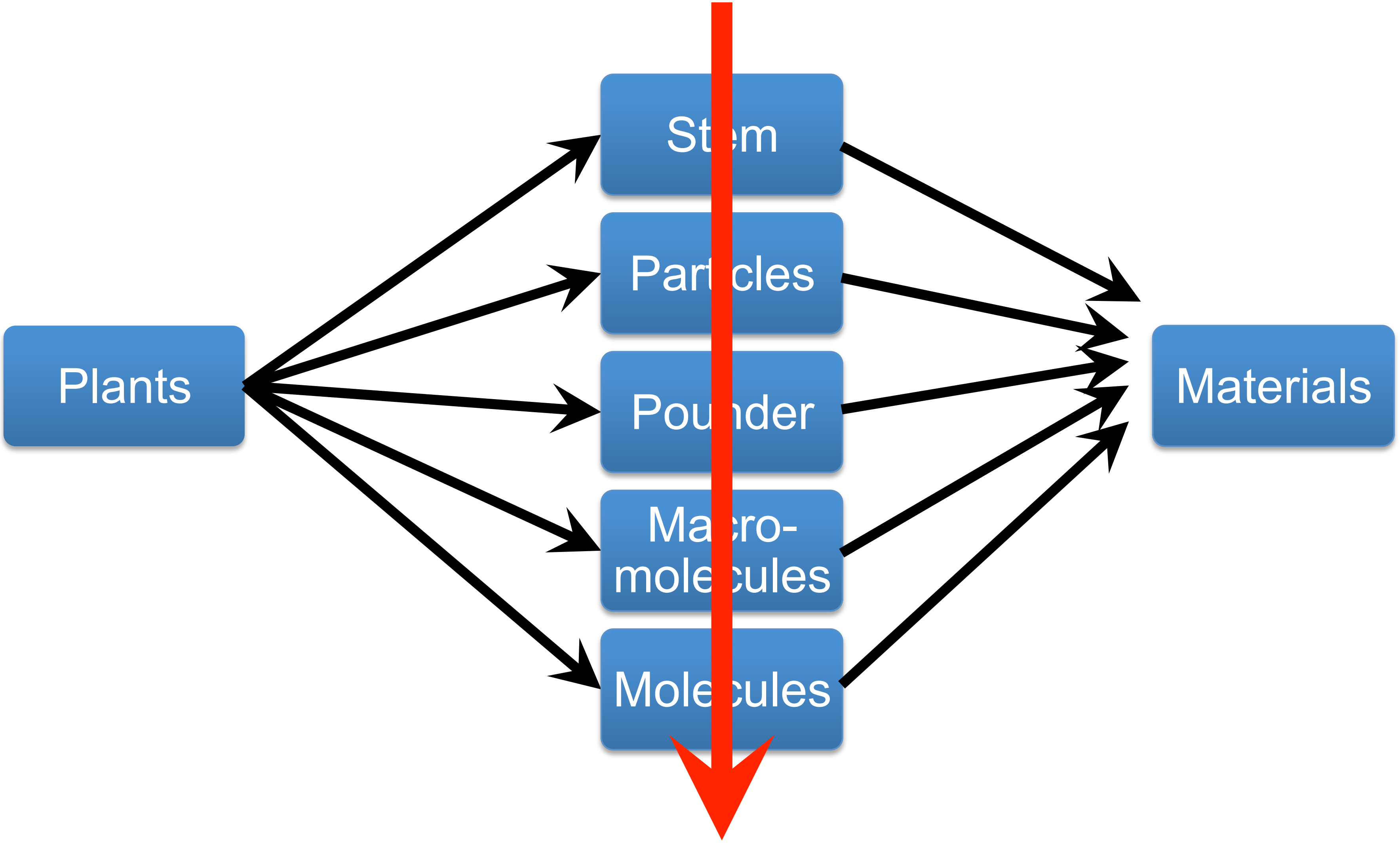




Thermal insulation



Composite materials



Increasing level of fragmentation

Various possibilities of composites …

- By increasing the level of fragmentation
  - Natural variability ↘
  - Performances ↗ or ↘
  - Cost of production ↗
  - Transformation energy ↗
  - Shape flexibility ↗
  - Standardisation ↗

Numerous composites materials

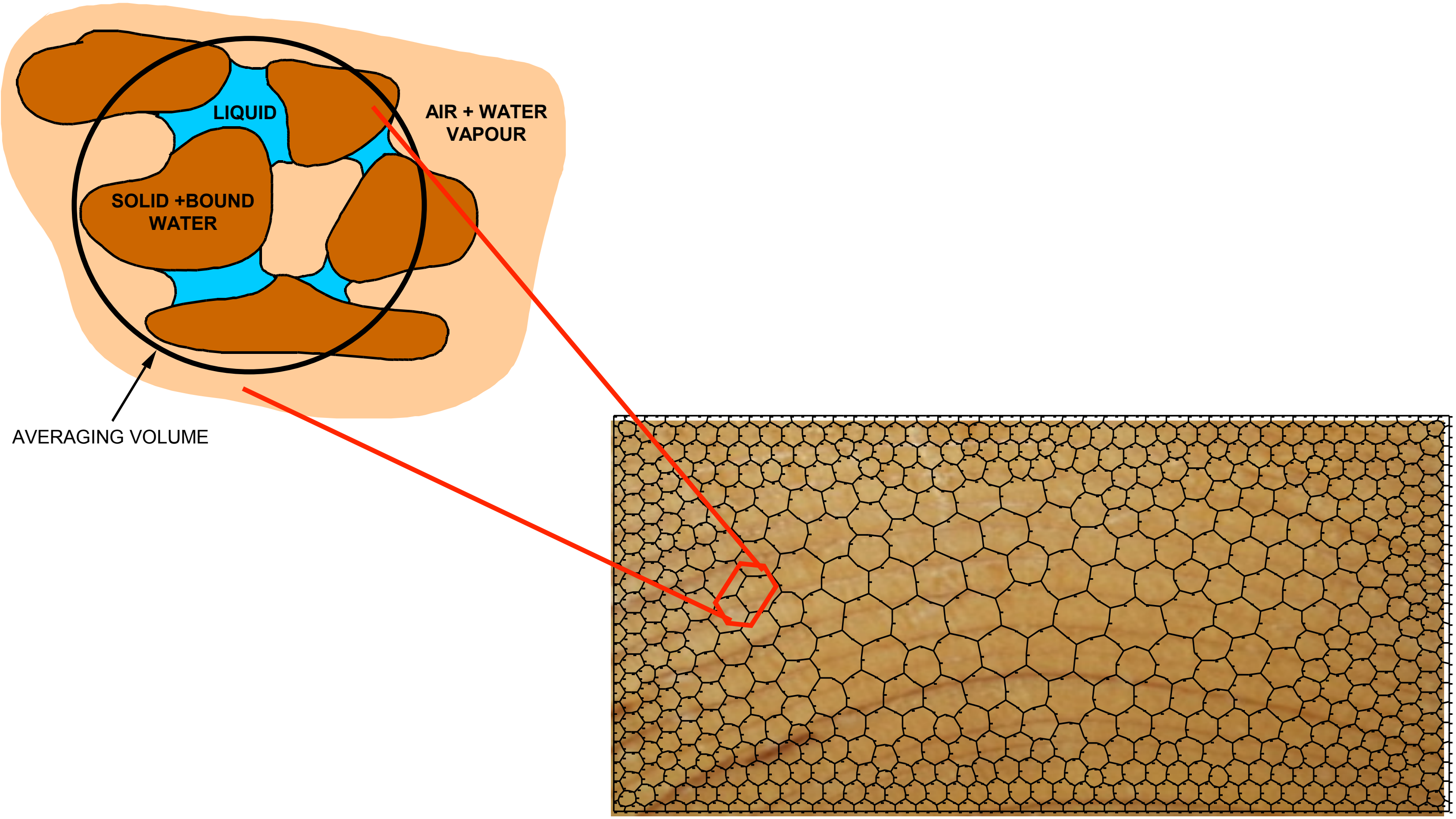
Transferts couplés chaleur/masse dans ces matériaux

Matériaux hygroscopiques

Stockage/déstockage de chaleur par changement d'état

- → "Moisture buffering effect"
- → Besoin de caractérisation, d'outils de prédiction des propriétés et d'outils de simulation

The macroscopic formulation



Comprehensive model

Water

$$\frac{\partial}{\partial t}\left(\varepsilon_w \rho_w + \varepsilon_g \rho_v + \bar{\rho}_b\right) + \nabla\cdot\left(\rho_w \bar{\mathbf{v}}_w + \rho_v \bar{\mathbf{v}}_g + \overline{\rho_b \mathbf{v}_b}\right) = \nabla\cdot\left(\rho_g \overline{\overline{\mathbf{D}}}_{\mathrm{eff}} \nabla\omega_v\right)$$

Enthalpy

$$\frac{\partial}{\partial t}\left(\varepsilon_w \rho_w h_w + \varepsilon_g (\rho_v h_v + \rho_a h_a) + \bar{\rho}_b \bar{h}_b + \rho_o h_s - \varepsilon_g P_g\right)$$

$$+ \nabla\cdot\left(\rho_w h_w \bar{\mathbf{v}}_w + (\rho_v h_v + \rho_a h_a)\bar{\mathbf{v}}_g + h_b \overline{\rho_b \mathbf{v}_b}\right)$$

$$= \nabla\cdot\left(\rho_g \overline{\overline{\mathbf{D}}}_{\mathrm{eff}} (h_v \nabla\omega_v + h_a \nabla\omega_a) + \overline{\overline{\lambda}}_{\mathrm{eff}} \nabla T\right) + \Phi$$

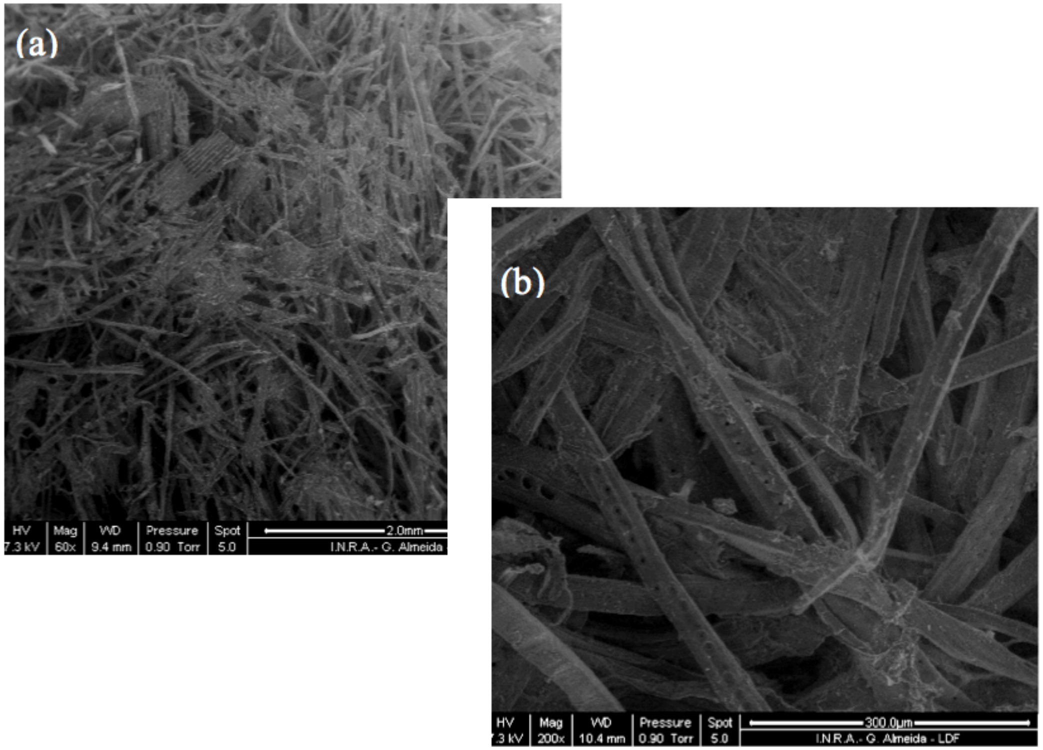
Air

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_a\right) + \nabla\cdot\left(\rho_a \bar{\mathbf{v}}_g\right) = \nabla\cdot\left(\rho_g \overline{\overline{\mathbf{D}}}_{\mathrm{eff}} \nabla\omega_a\right)$$

Generalised Darcy's law

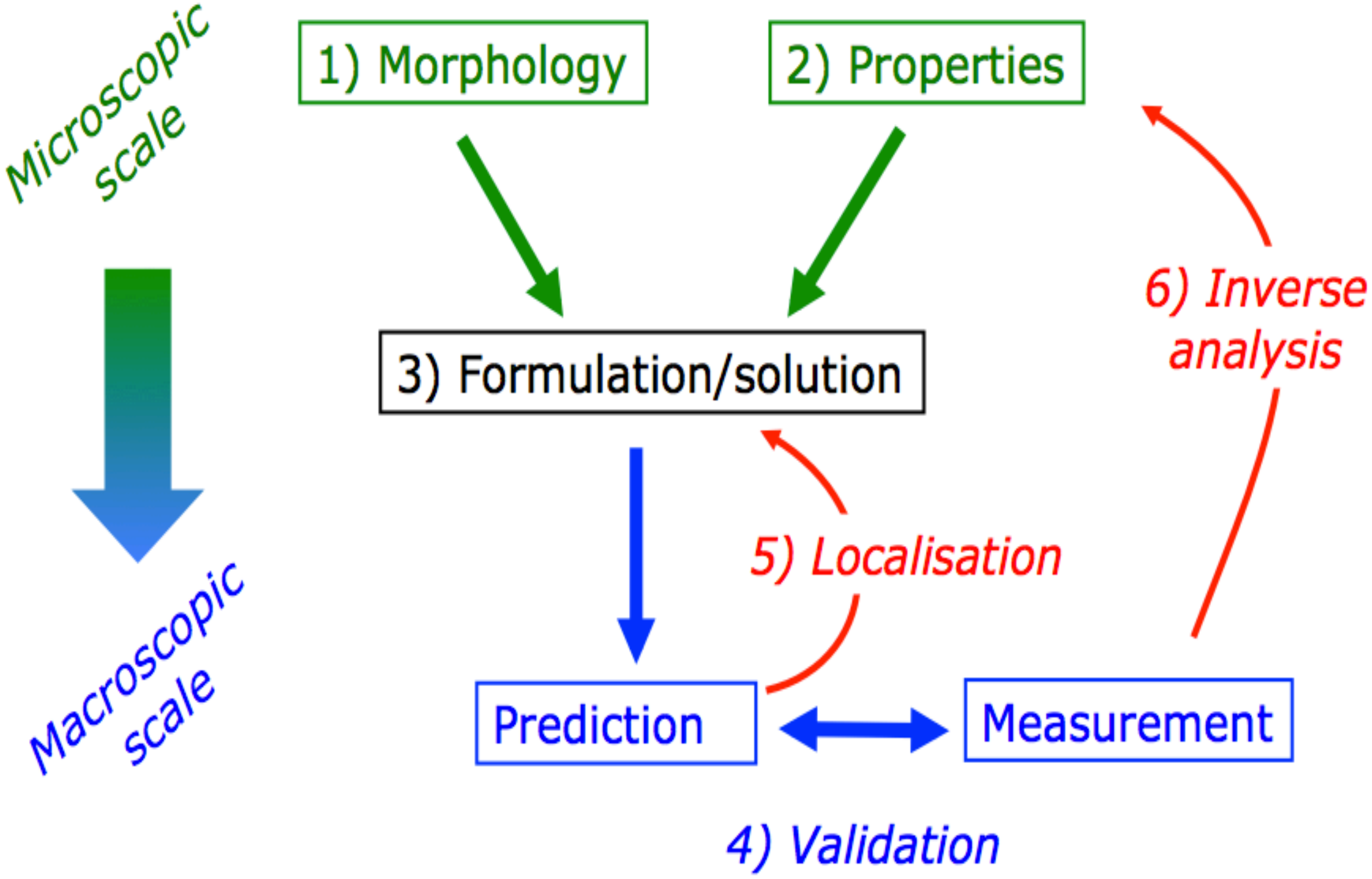
$$\bar{\mathbf{v}}_\ell = -\frac{\overline{\overline{\mathbf{K}}}_\ell \overline{\overline{\mathbf{k}}}_\ell}{\mu_\ell} \nabla\varphi_\ell \quad , \quad \nabla\varphi_\ell = \nabla P_\ell - \rho_\ell g \nabla\chi \qquad \text{where} \quad \ell = w, g$$

Parois composites

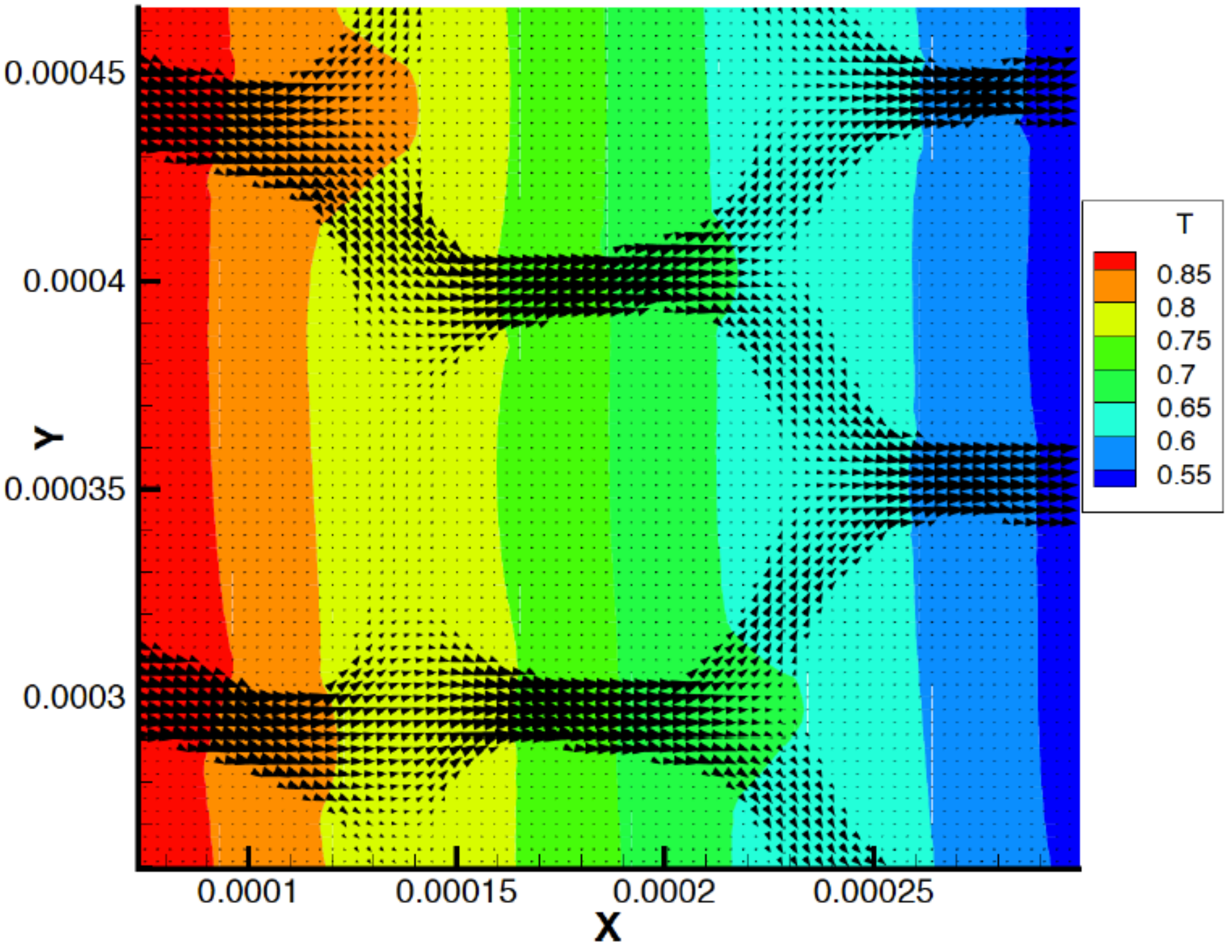


Clichés ESEM (G. Almeida)

Up-scaling

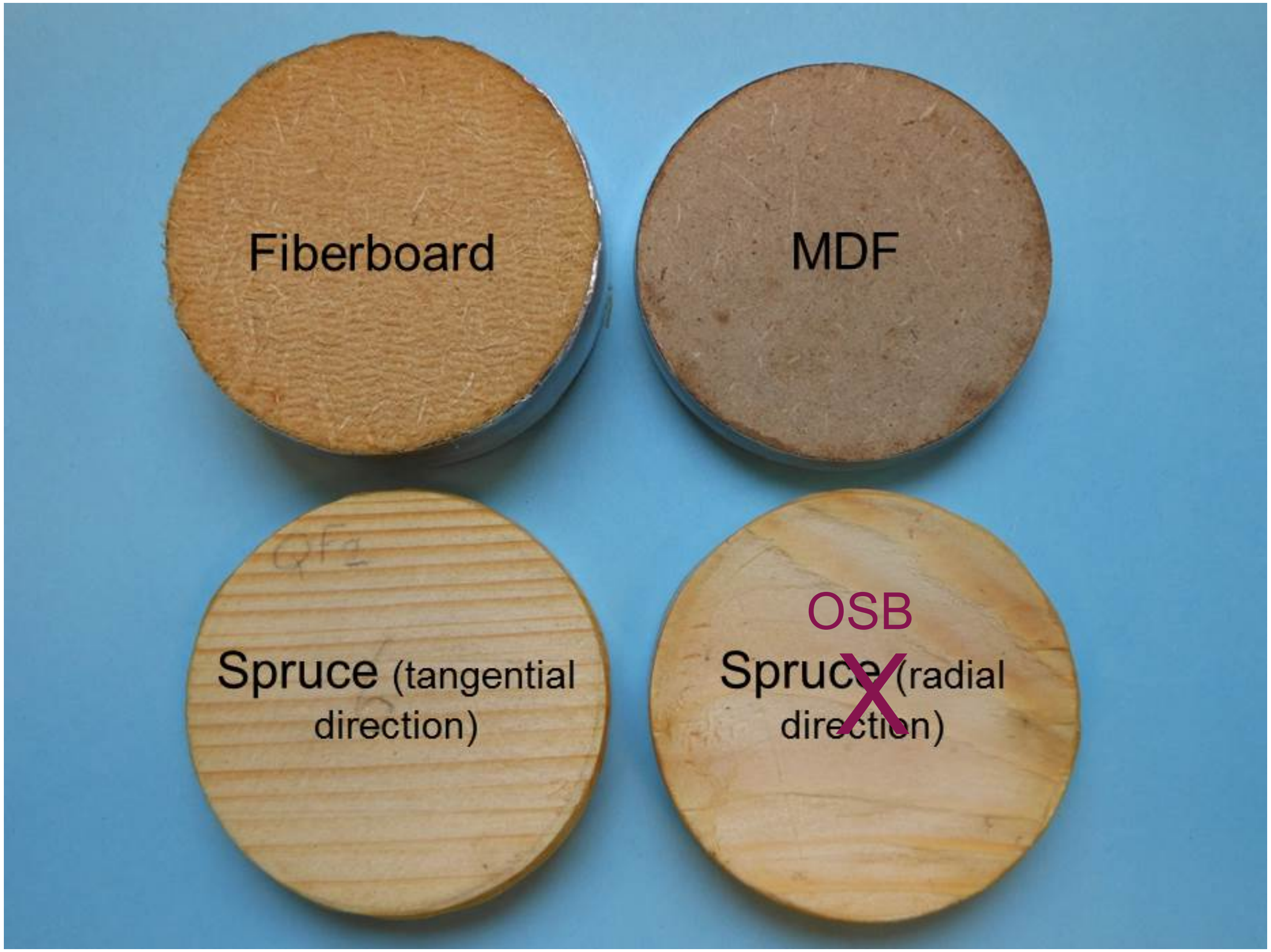

Microscopic scale
1) Morphology
2) Properties
3) Formulation/solution
6) Inverse analysis
5) Localisation
Macroscopic scale
Prediction
Measurement
4) Validation

Prédiction par changement d'échelle : exemple de modélisation des transferts par Lattice Bolzmann



Perré et al., Annals Forest Sci., accepted

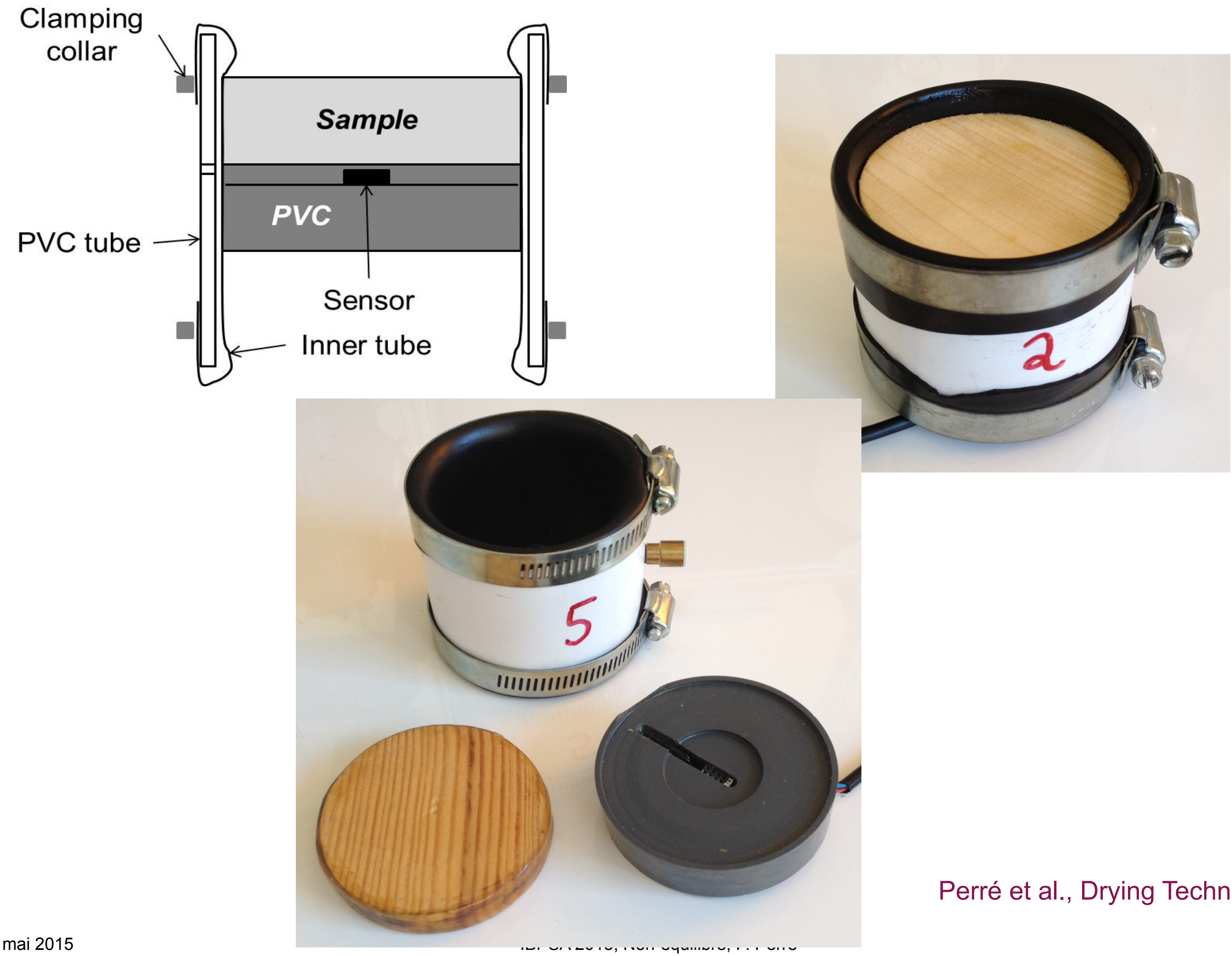
Caractérisation expérimentale



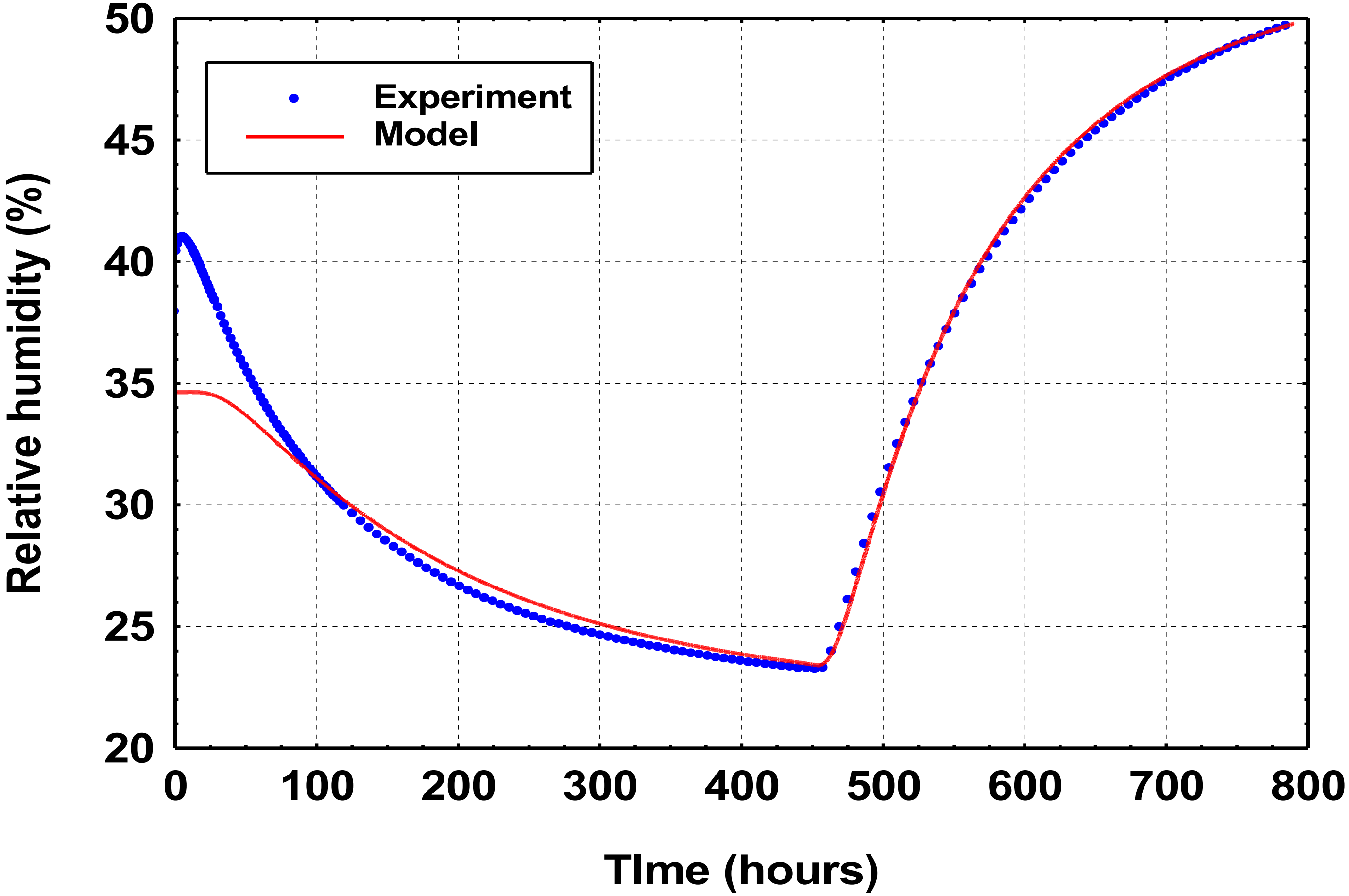
Principes de mesure = suivi de l'effet d'une perturbation extérieure

- Régime permanent (coupelle) : on impose un saut de HR et on mesure le flux qui en résulte en régime permanent,
- Régime transitoire : on soumet l'échantillon à une variation brusque de HR et on mesure l'évolution de sa masse,
- Sollicitations moins maitrisées → méthodes inverses

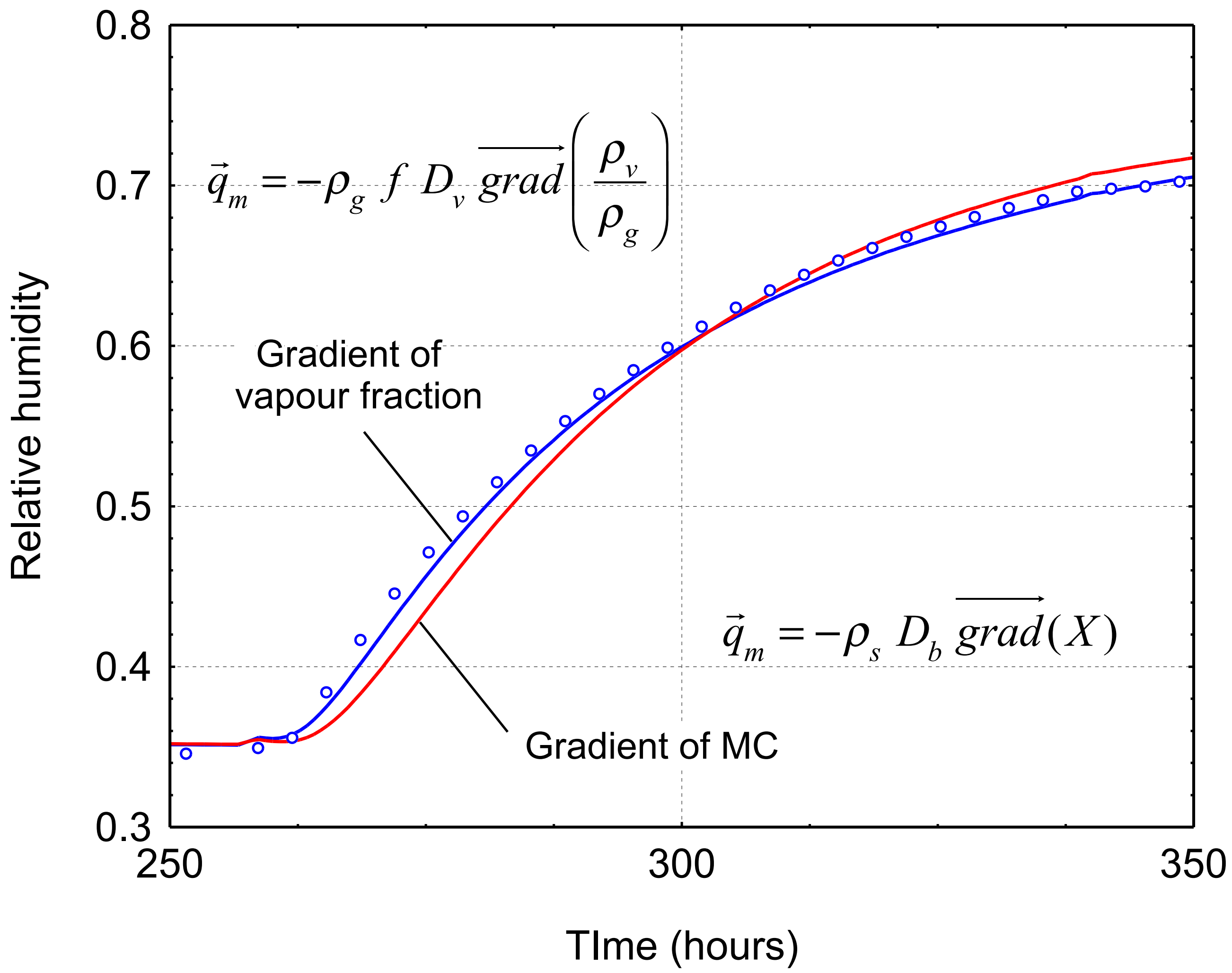
Mesure de HR en face arrière



Perré et al., Drying Technology, in press


50
45
40
35
30
25
20
0
100
200
300
400
500
600
700
800
Relative humidity (%)
TIme (hours)
Experiment
Model

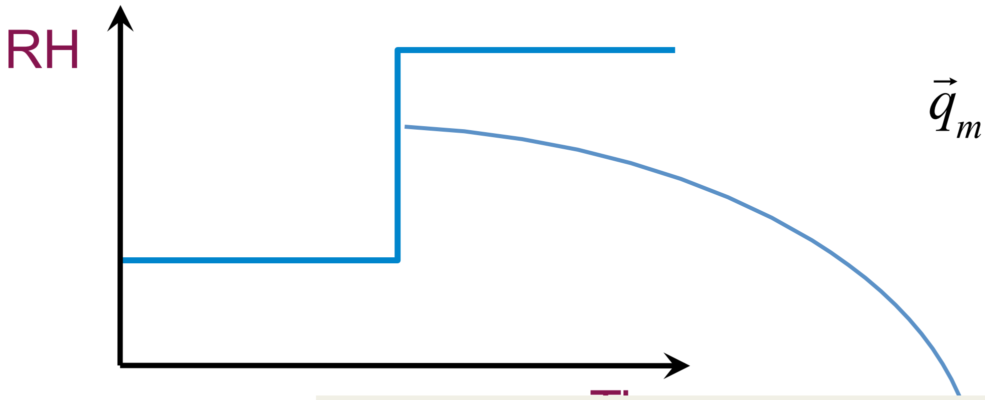
Choice of the driving force for diffusion (Spruce Radial direction)



$$\vec{q}_m = -\rho_g \, f \, D_v \, \overrightarrow{grad}\left(\frac{\rho_v}{\rho_g}\right)$$

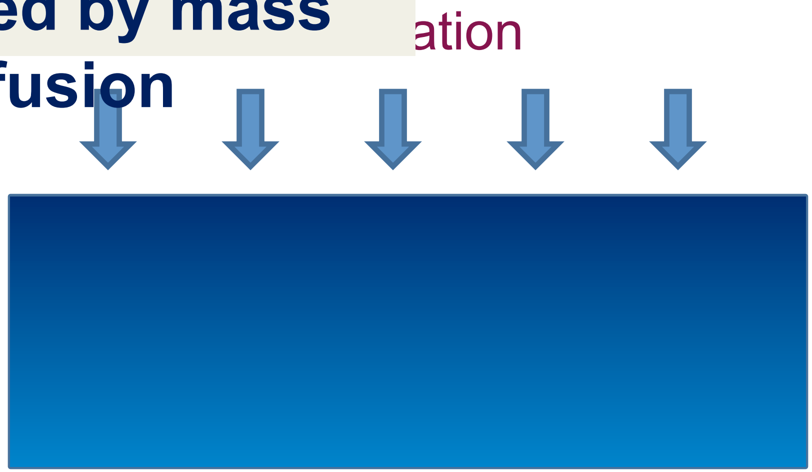
$$\vec{q}_m = -\rho_s \, D_b \, \overrightarrow{grad}(X)$$

Mass transfer only

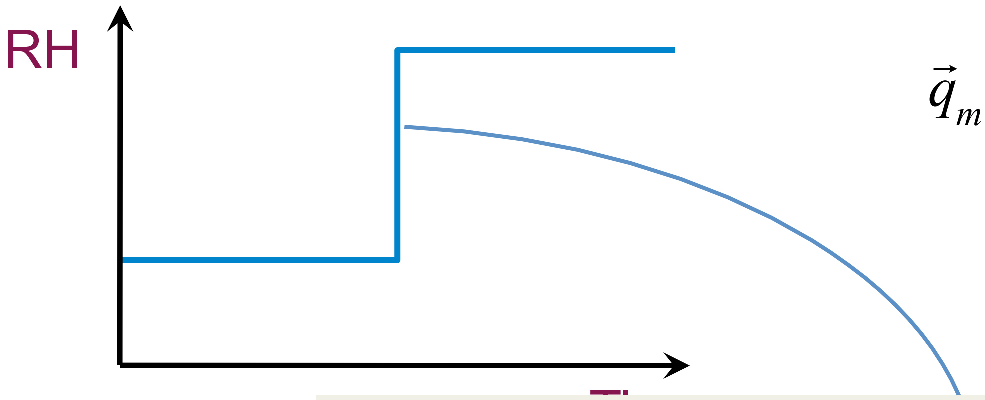


$$\vec{q}_m = -\rho_s \, D_b \, \overrightarrow{grad}(X)$$

Time constant controlled by mass diffusion



H & M transfer coupling

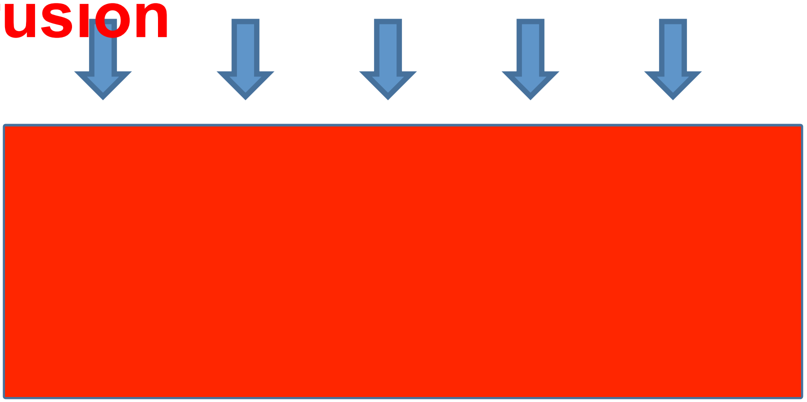


$$\vec{q}_m = -\rho_g \; f \; D_v \; \overrightarrow{grad}\left(\frac{\rho_v}{\rho_g}\right)$$

$$P_v = a(X,T)P_{vs}(T)$$

Time constant controlled by thermal diffusion

ation

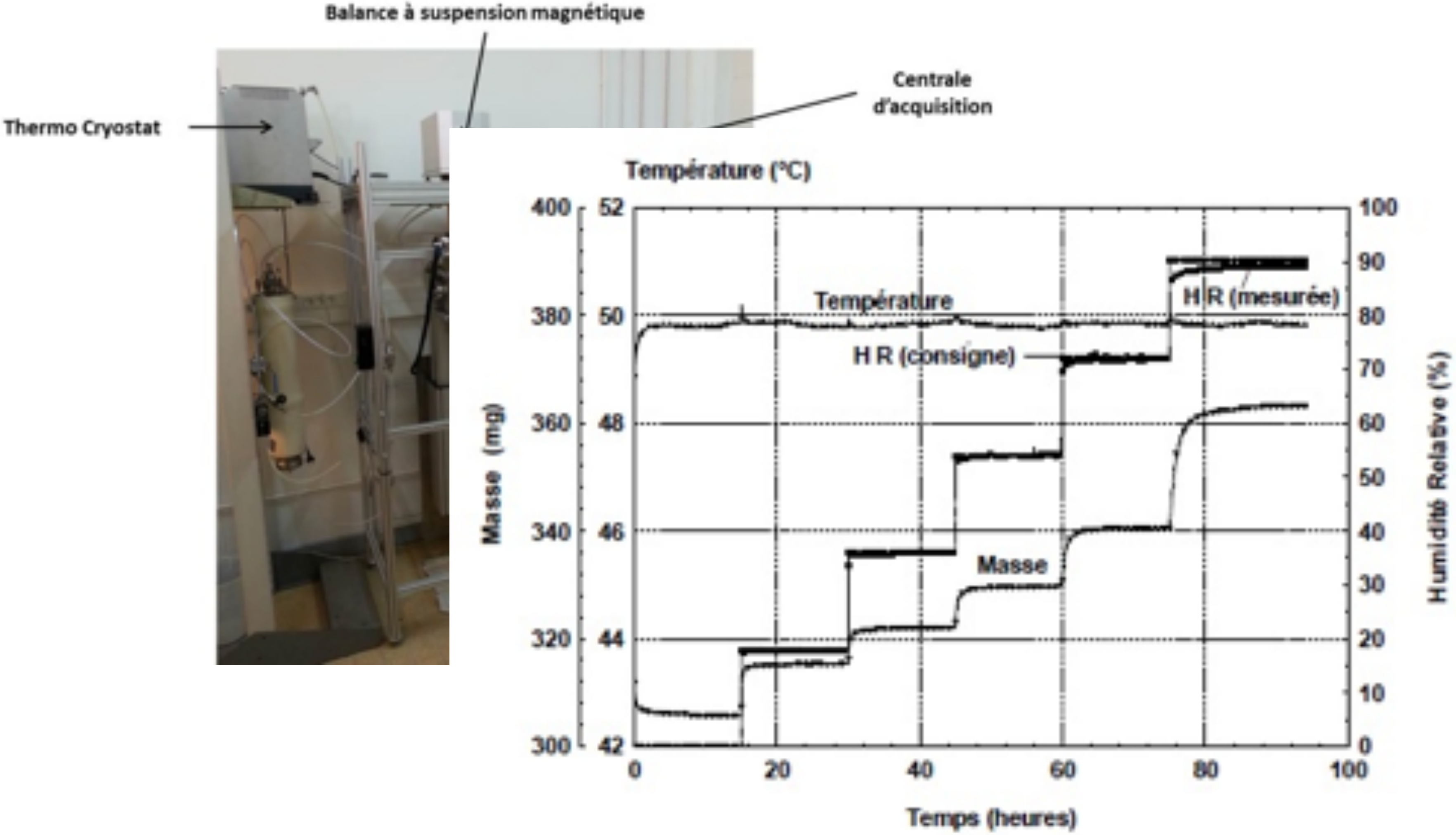


Some results

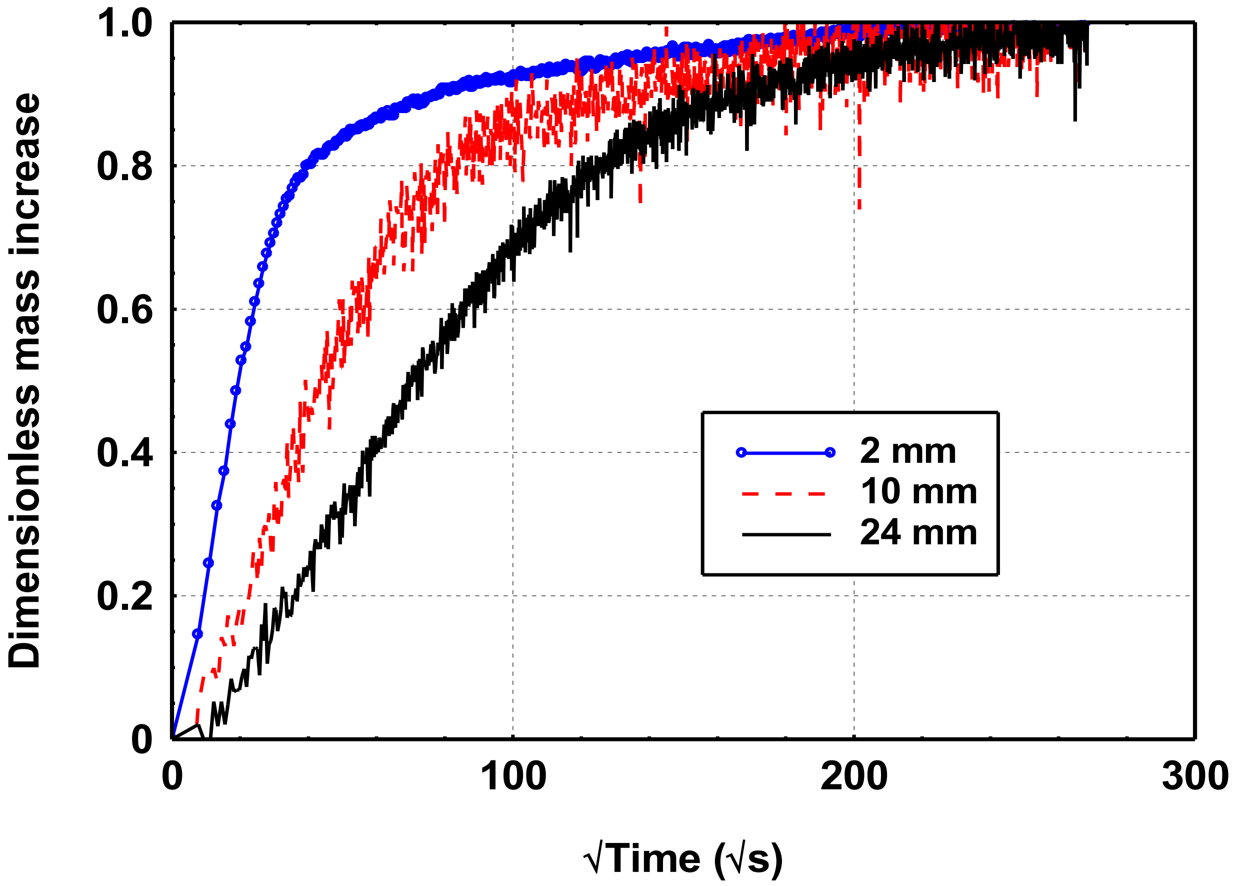
Sample		*f*
Spruce	Radial 1	0.0142
	Radial 2	0.0123
	Tangential 1	0.0182
	Tangential 2	0.0187
MDF 1		0.297
MDF 2		0.238
LDF		**1.45**

Perré et al., in press

Experimental device

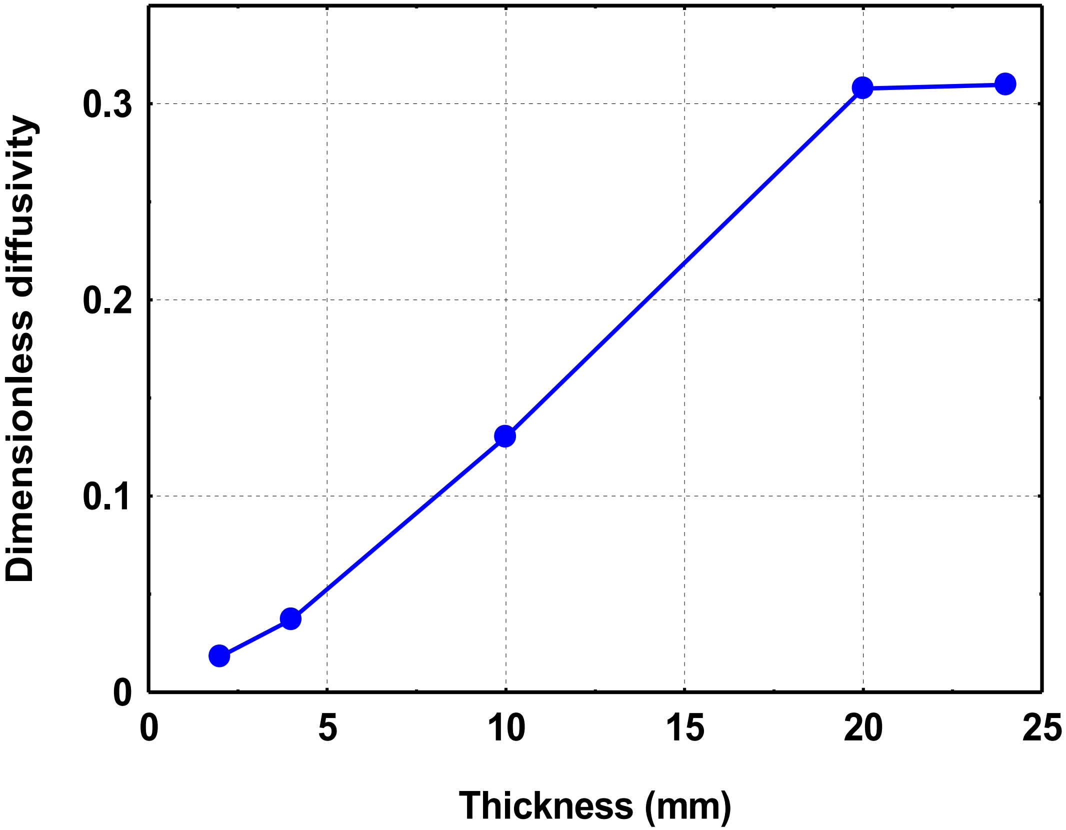


Experimental results : effect of thickness



Coefficient de diffusion

$$\frac{\Delta m(t)}{\left|\Delta m\right|_{total}} = \frac{4}{e} \cdot \sqrt{\frac{D}{\pi}} \cdot \sqrt{t}$$

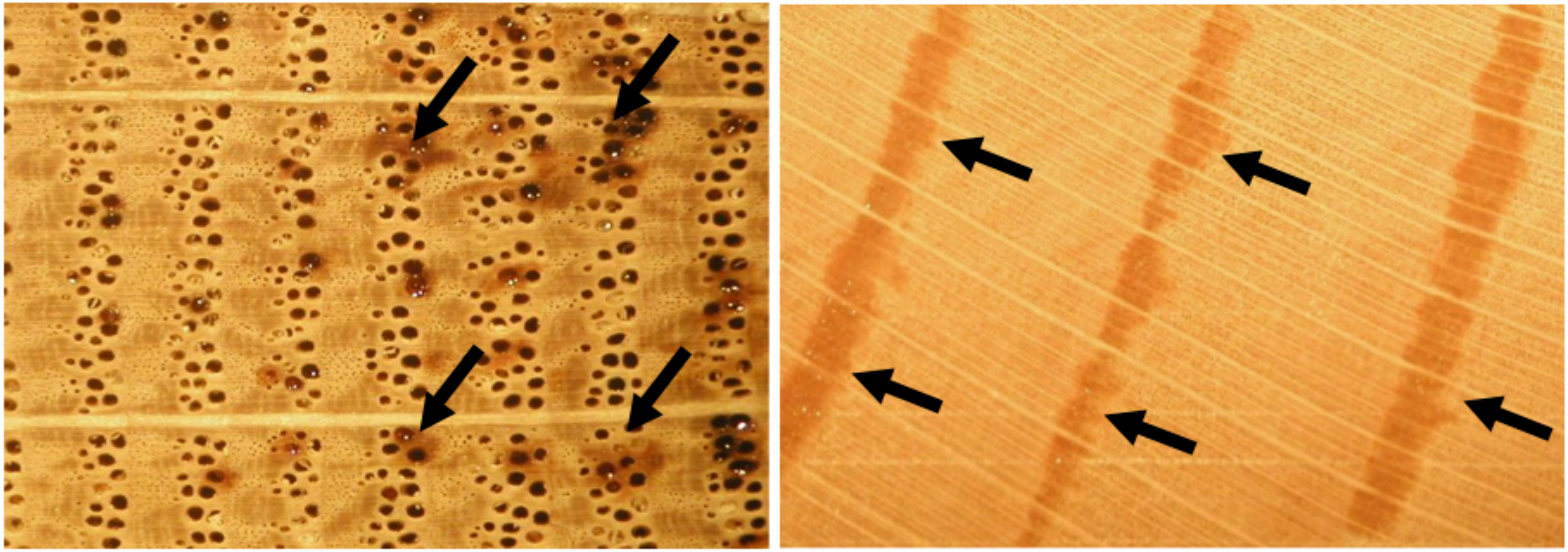


Almeida, Rémond, Perré, Proc. Int. Drying Symposium, 2010

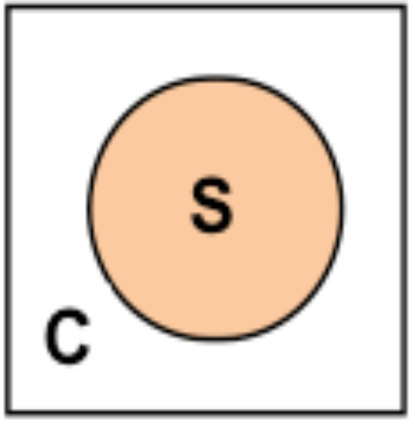
Le comportement macroscopique non-fickien est expliqué par un effet de double échelle

- Une constante de temps dépend de la diffusion "rapide" dans la phase conductrice et connexe (macroscopique)
- Une autre constante de temps est liée à la diffusion "lente" dans la phase de stockage (microscopique)
- Selon la configuration (épaisseur, densité, conditions aux limites), l'une de ces constantes de temps contrôle la réponse macroscopique ou les deux phénomènes interagissent

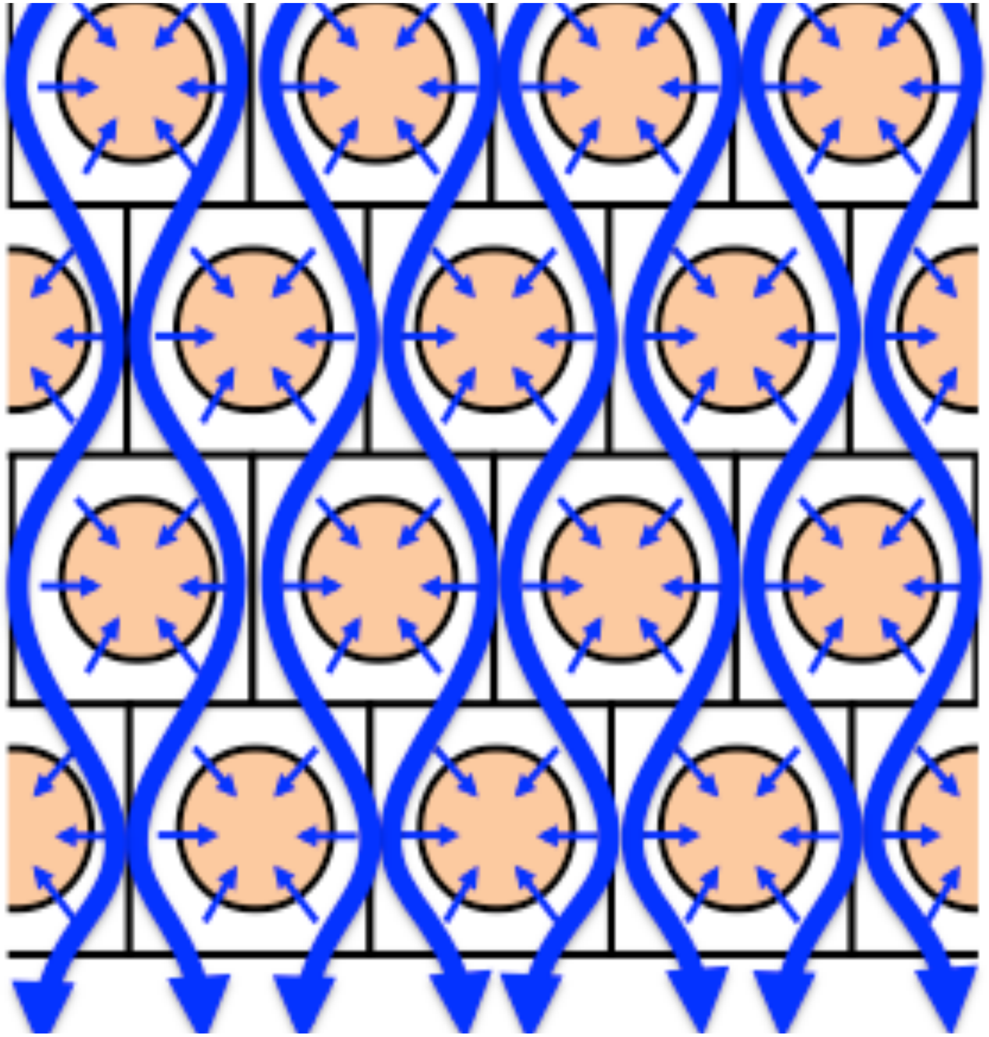
Un exemple visuel : imbibition de liquide dans le bois (L)



Dual scale effects



S : storage phase
C : conductive phase



Micro-modèles distribués (Schowalter, 1993) et au-delà…

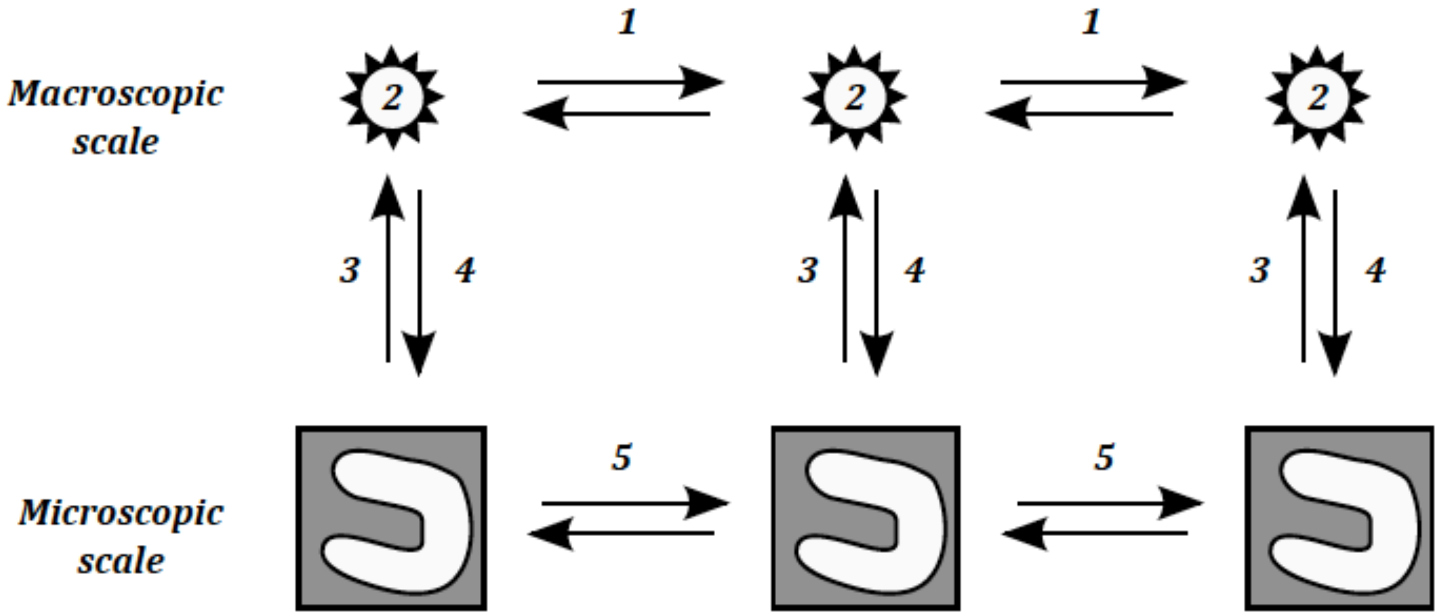


Figure 1.1: Possible interactions within and between the macroscopic and microscopic scales for the balance equations.

Carr E., Turner I., Perré P., Multiscale Modeling & Simulation, 2013

Formulation

Microscopic scale

Moisture conservation

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\varepsilon_w^S\rho_w^S + \varepsilon_g^S\rho_v^S + \overline{\rho_b}^S\right) + \nabla_y\cdot\left(\rho_w^S\bar{\mathbf{v}}_w^S + \rho_v^S\bar{\mathbf{v}}_g^S + \overline{\rho_b\mathbf{v}_b}^S\right)\\&= \nabla_y\cdot\left(\rho_g^S\overline{\overline{\mathbf{D}}}_{eff}^S\nabla_y\omega_v^S\right)\quad y\in S_x,\ x\in\Omega\end{aligned}\tag{1}$$

Energy conservation

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\varepsilon_w^S\rho_w^S h_w^S + \varepsilon_g^S(\rho_v^S h_v^S + \rho_a^S h_a^S) + \overline{\rho_b}^S\bar{h}_b^S + \varepsilon_s^S\rho_s^S h_s^S - \varepsilon_g^S P_g^S\right)\\&+\nabla_y\cdot\left(\rho_w^S h_w^S\bar{\mathbf{v}}_w^S + (\rho_v^S h_v^S + \rho_a^S h_a^S)\bar{\mathbf{v}}_g^S + h_b^S\overline{\rho_b\mathbf{v}_b}^S\right)\\&= \nabla_y\cdot\left(\rho_g^S\overline{\overline{\mathbf{D}}}_{eff}^S(h_v^S\nabla_y\omega_v^S + h_a^S\nabla_y\omega_a^S) + \overline{\overline{\lambda}}_{eff}^S\nabla_y T^S\right)\quad y\in S_x,\ x\in\Omega\end{aligned}\tag{2}$$

Perré P., Drying Technology, 2010

Formulation

Macroscopic scale

Moisture conservation

$$\frac{\partial}{\partial t}(\varepsilon_g^C \rho_v^C) + \nabla_x \cdot (\rho_v^C \bar{\mathbf{v}}_g^C) = \nabla_x \cdot \left(\rho_g^C \overline{\overline{\mathbf{D}}}_{eff}^C \nabla_x \omega_v^C \right) + Q_v(t,x) \quad x \in \Omega \tag{4}$$

Energy conservation

$$\begin{aligned} &\frac{\partial}{\partial t}\left(\varepsilon_g^C(\rho_v^C h_v^C + \rho_a^C h_a^C)\right) + \nabla_x \cdot \left((\rho_v^C h_v^C + \rho_a^C h_a^C)\bar{\mathbf{v}}_g^C\right) \\ &= \nabla_x \cdot \left(\rho_g^C \overline{\overline{\mathbf{D}}}_{eff}^C (h_v^C \nabla_x \omega_v^C + h_a^C \nabla_x \omega_a^C) + \overline{\overline{\lambda}}_{eff}^C \nabla_x T^C \right) + Q_h(t,x) \quad x \in \Omega \end{aligned} \tag{5}$$

Perré P., Drying Technology, 2010

Formulation

Coupling between scales

Moisture conservation

$$\overline{\overline{\lambda}}^S_{eff} \nabla_y T^S \cdot \vec{n} = h^S_h \left[T^S(t,x,y) - T^C(t,x) \right] \quad y \in \partial S_x, \; x \in \Omega \tag{7}$$
$$Q_h(t,x) = \frac{1}{|Y|} \int_\Gamma \overline{\overline{\lambda}}^S_{eff} \nabla_y T^S \cdot \vec{n} \, dS \quad x \in \Omega$$

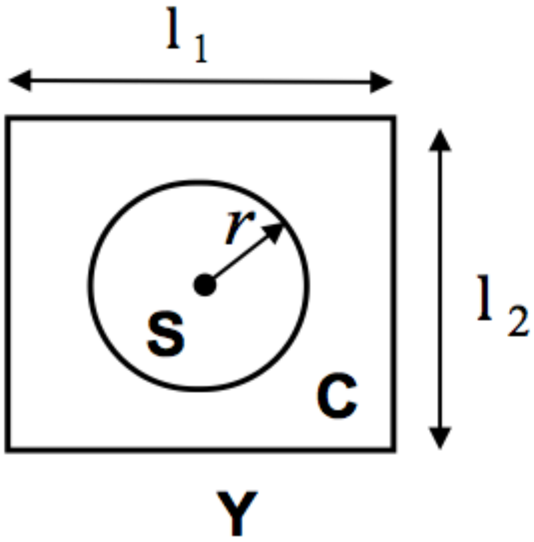
Energy conservation

$$\rho^S_g \overline{\overline{\mathbf{D}}}^S_{eff} \nabla_y \omega^S_v \cdot \vec{n} = h^S_m \rho^S_g \left(\omega^S_v(t,x,y) - \omega^C_v(t,x) \right) \quad y \in \partial S_x, \; x \in \Omega \tag{8}$$
$$Q_v(t,x) = \frac{1}{|Y|} \int_\Gamma \rho^S_g \overline{\overline{\mathbf{D}}}^S_{eff} \nabla_y \omega^S_v \cdot \vec{n} \, dS \quad x \in \Omega$$

Perré P., Drying Technology, 2010

Application à la diffusion dans un milieu fibreux

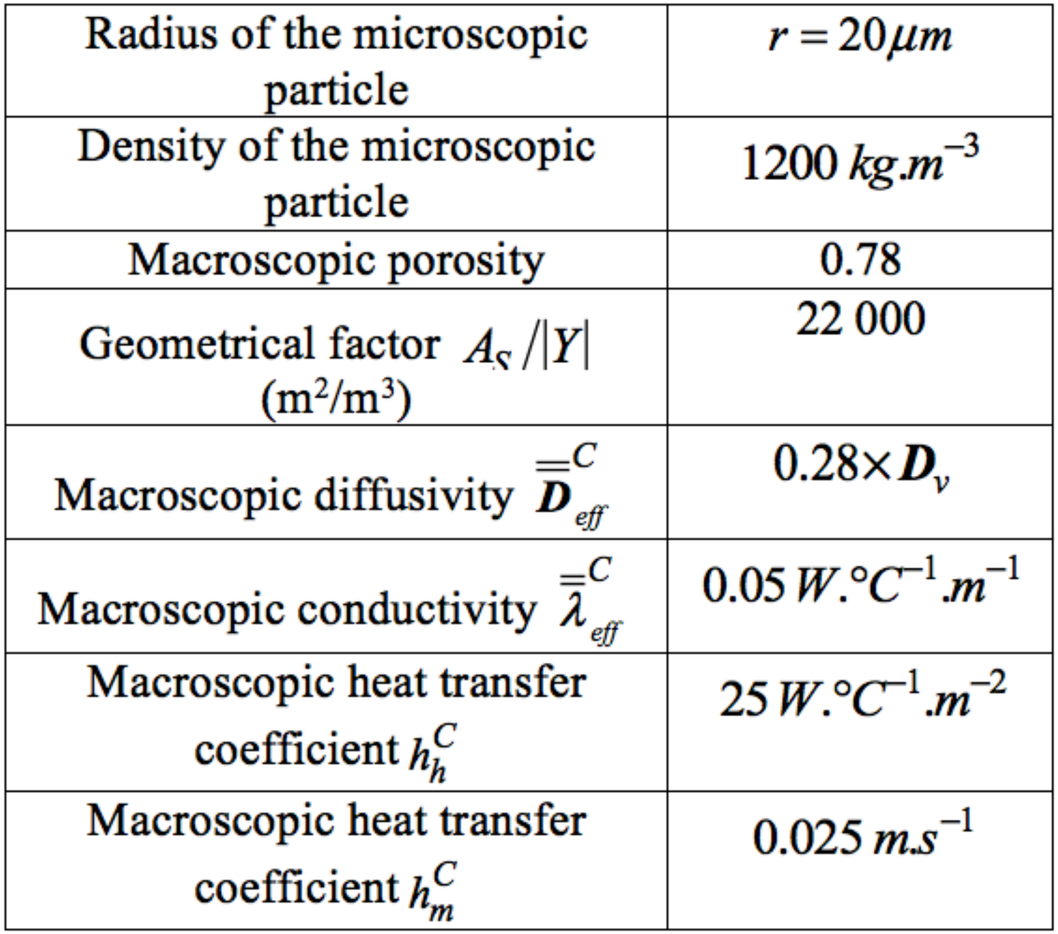
Choix du VER



$$\phi_{mac} = \frac{\pi r^2}{l_1 \times l_2}$$

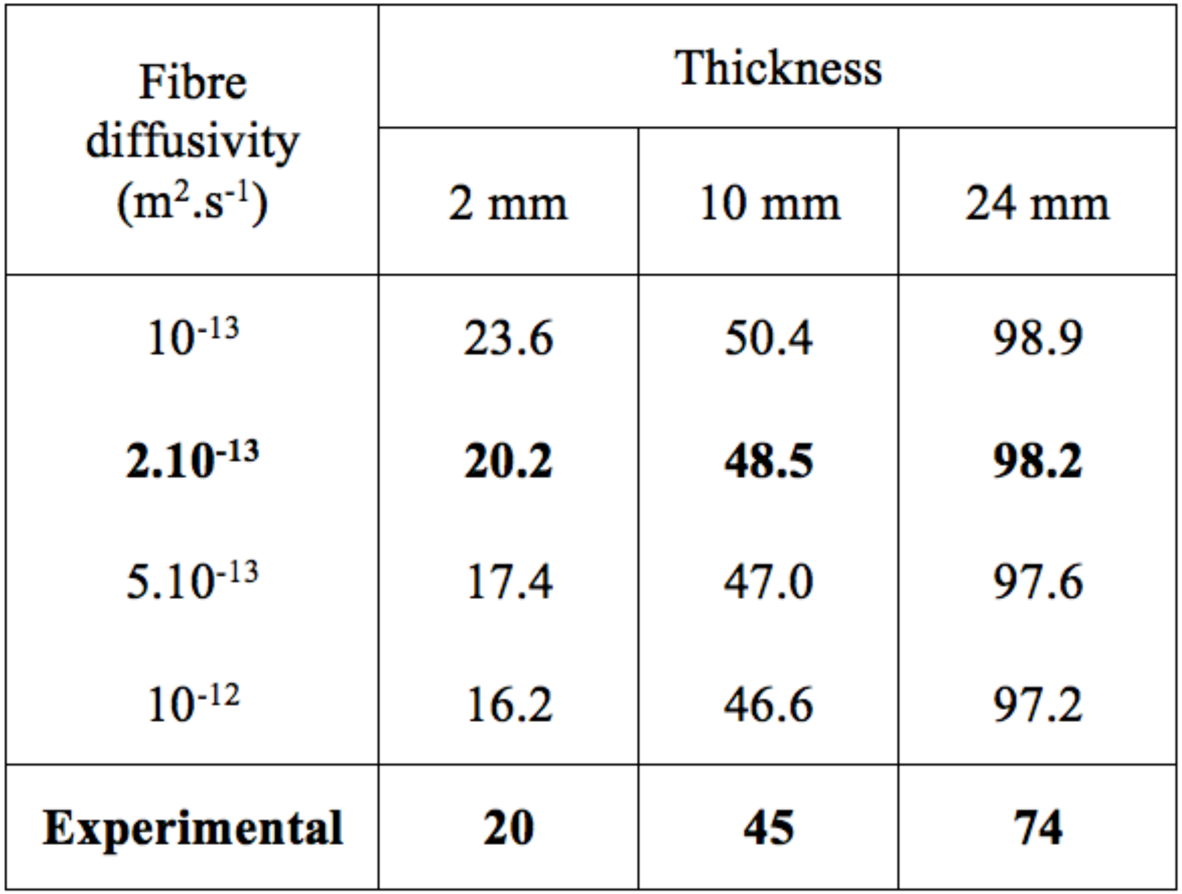
Particle volume	$\pi r^2 L_0$
Exchange surface	$2\pi r L_0$
Volume of the unit cell	$\frac{\pi r^2 L_0}{1-\phi_{mac}}$
Geometrical factor $A_S / \lvert Y \rvert$ (m²/m³)	$\frac{2(1-\phi_{mac})}{r}$

Paramètres physiques



Radius of the microscopic particle	$r = 20 \mu m$
Density of the microscopic particle	$1200\ kg.m^{-3}$
Macroscopic porosity	0.78
Geometrical factor $A_S / \lvert Y \rvert$ (m^2/m^3)	22 000
Macroscopic diffusivity $\overline{\overline{\boldsymbol{D}}}^{C}_{eff}$	$0.28 \times \boldsymbol{D}_v$
Macroscopic conductivity $\overline{\overline{\lambda}}^{C}_{eff}$	$0.05\ W.°C^{-1}.m^{-1}$
Macroscopic heat transfer coefficient h_h^C	$25\ W.°C^{-1}.m^{-2}$
Macroscopic heat transfer coefficient h_m^C	$0.025\ m.s^{-1}$

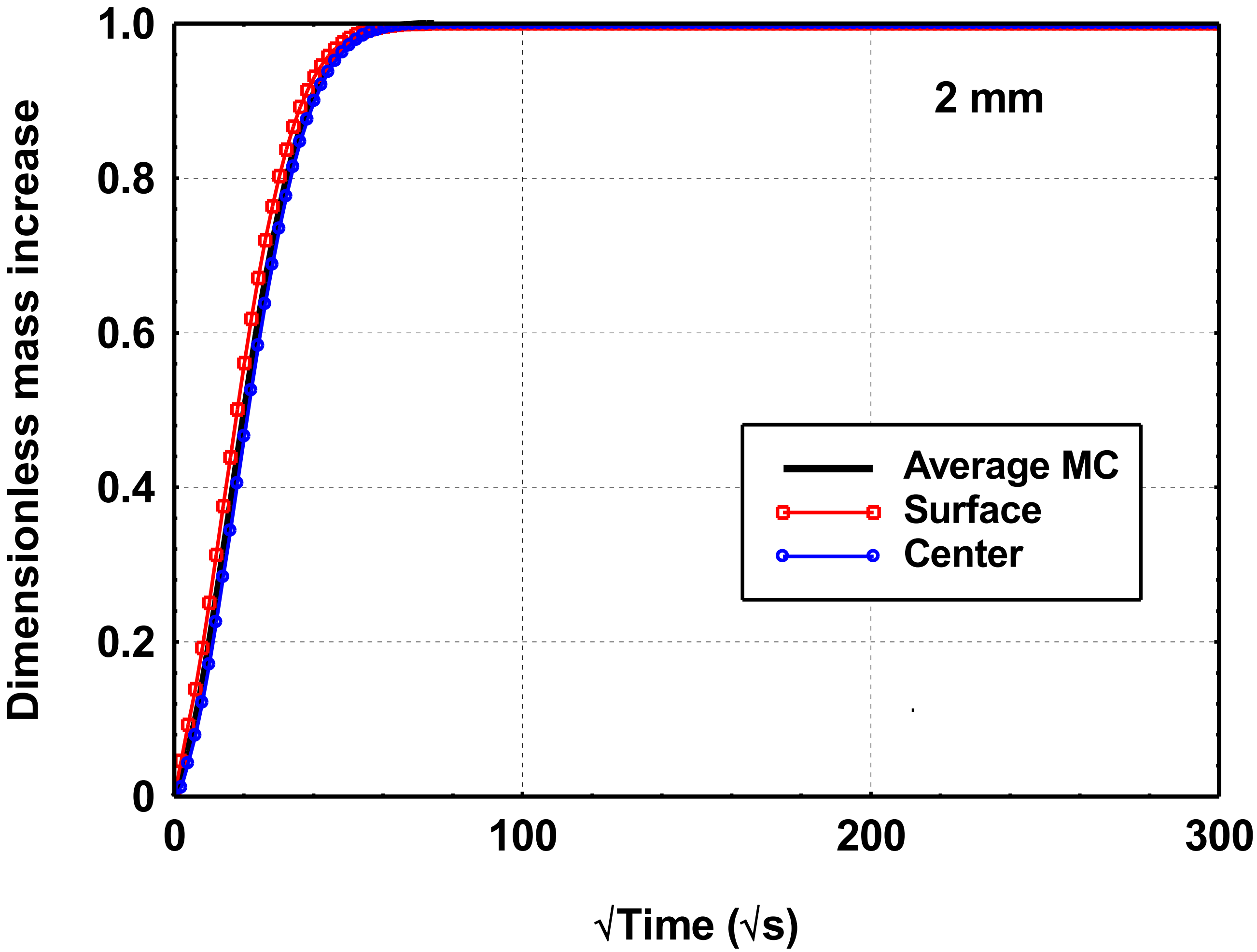
Cohérence modèle/expérience



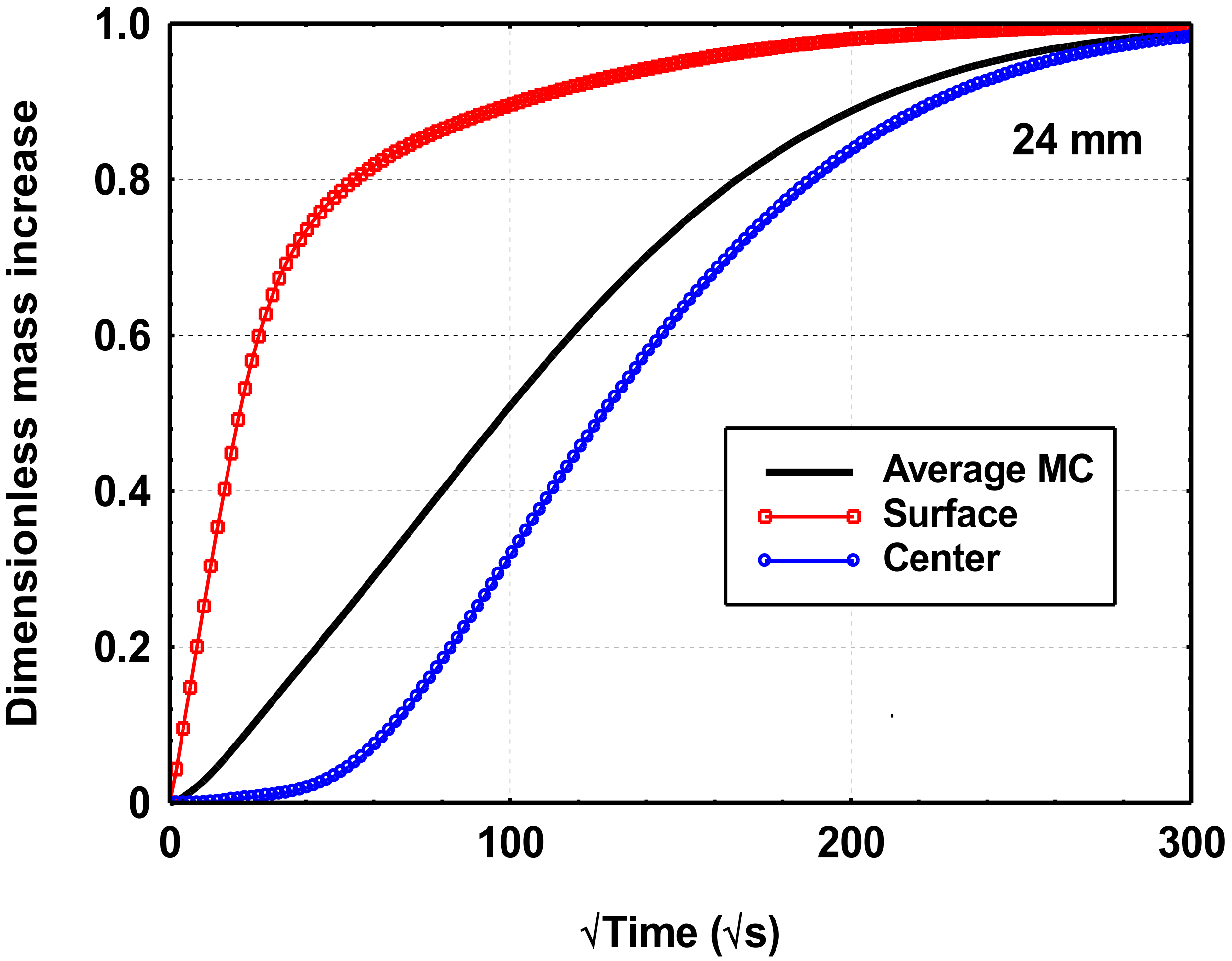
Fibre diffusivity ($m^2.s^{-1}$)	Thickness		
	2 mm	10 mm	24 mm
10^{-13}	23.6	50.4	98.9
2.10^{-13}	**20.2**	**48.5**	**98.2**
5.10^{-13}	17.4	47.0	97.6
10^{-12}	16.2	46.6	97.2
Experimental	**20**	**45**	**74**

Almeida, Rémond, Perré, Proc. Int. Drying Symposium, 2010

Dual scale effects

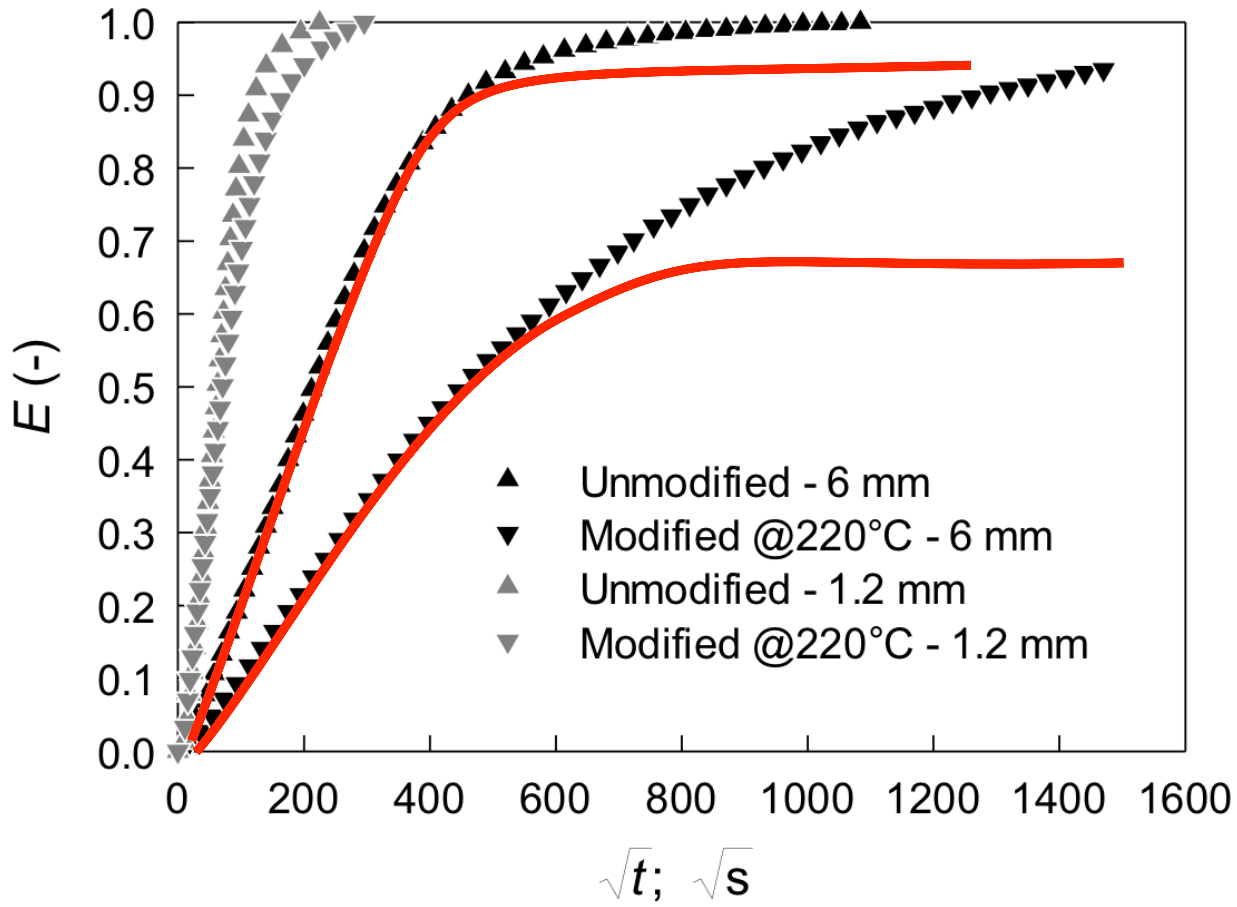


Dual scale effects



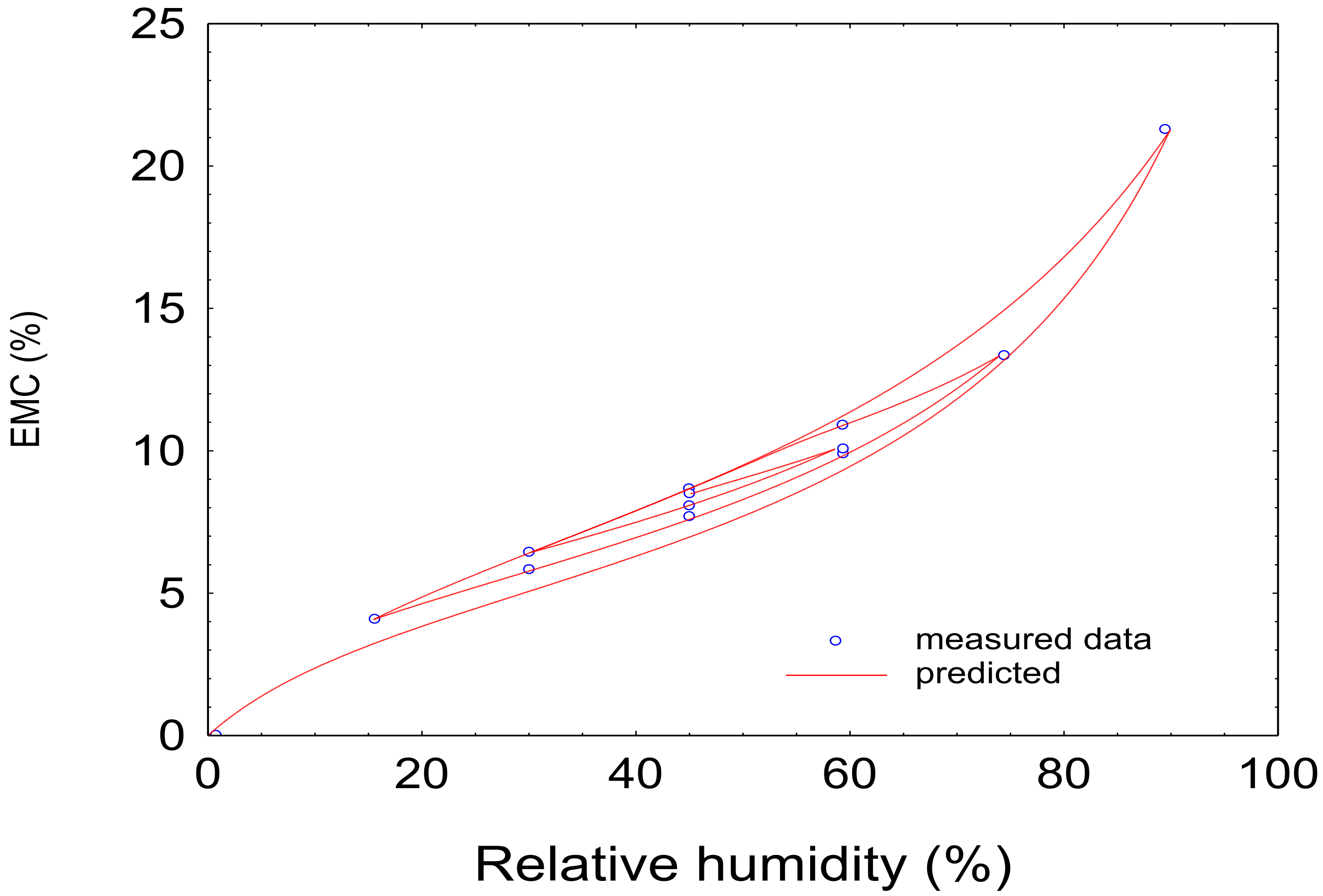
Autres phénomènes responsables du non-équilibre local

Evidence of non-Fickian behavior in thermally modified wood.



Olek et al., submitted

Hystérésis de sorption : mesures et modélisation



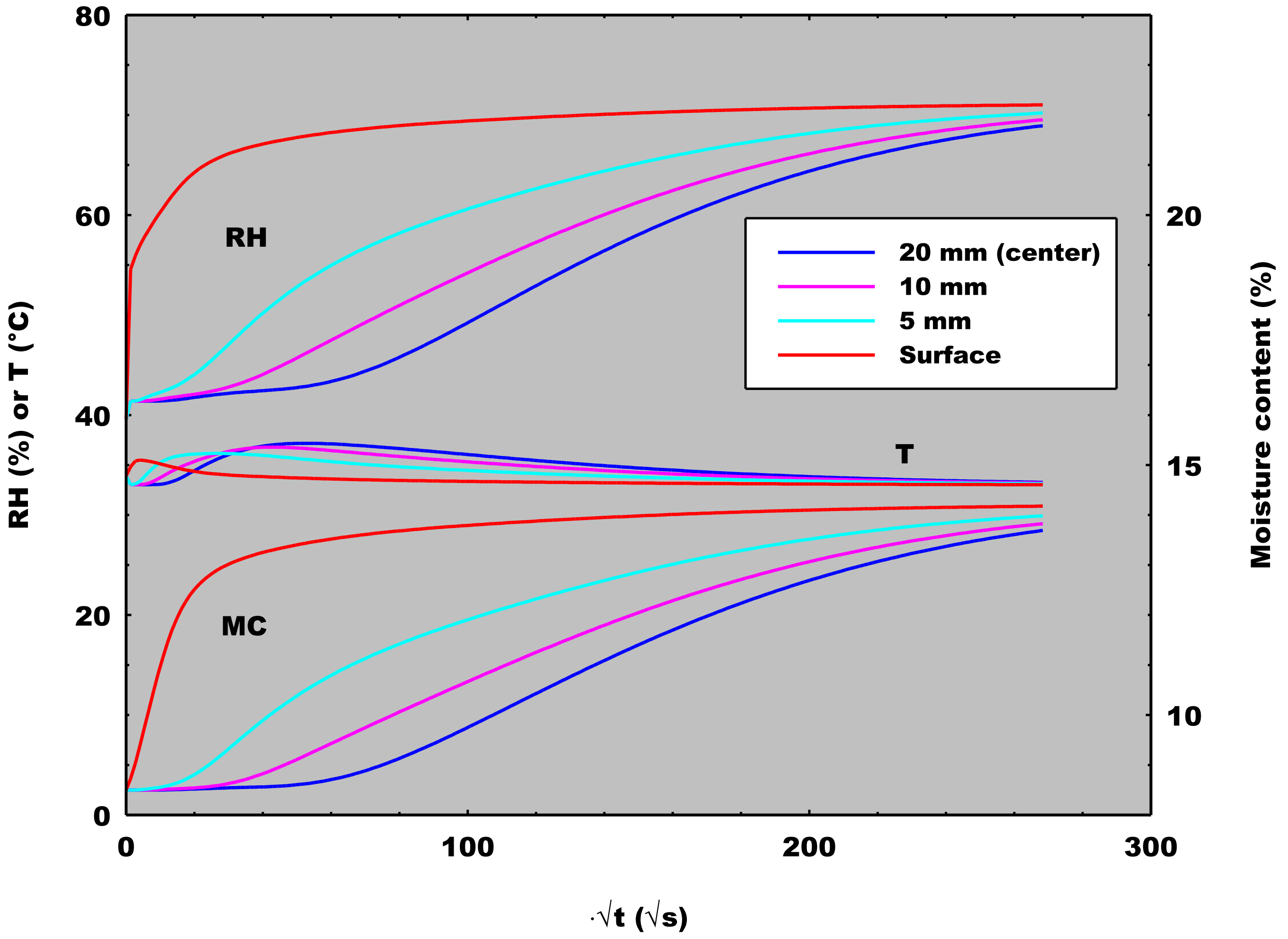
Rémond, Almeida, Perré, en préparation

Simulations : effects of dual-scale and relaxation

- LDF panel (20 mm thick)
- Sudden change in RH
- 3 case studies:
    - Test 1 : $D_{fibres} = 10^{-12}$ m²/s
    - Test 2 : $D_{fibres} = 10^{-13}$ m²/s
    - Test 3 : $D_{fibres} = 10^{-13}$ m²/s and relaxation

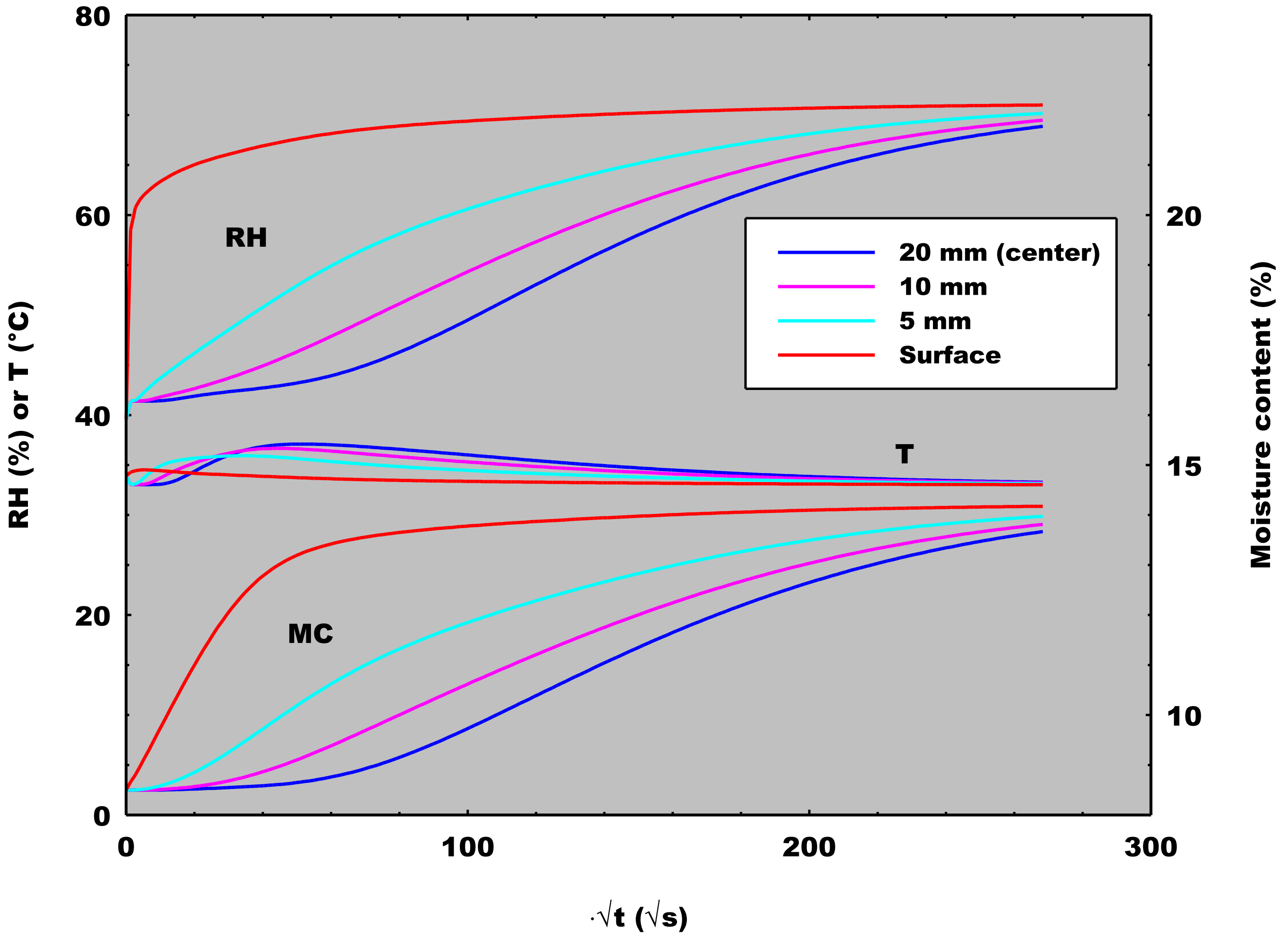
      (α=15% and τ=0.3 10^5 s)

Test 1

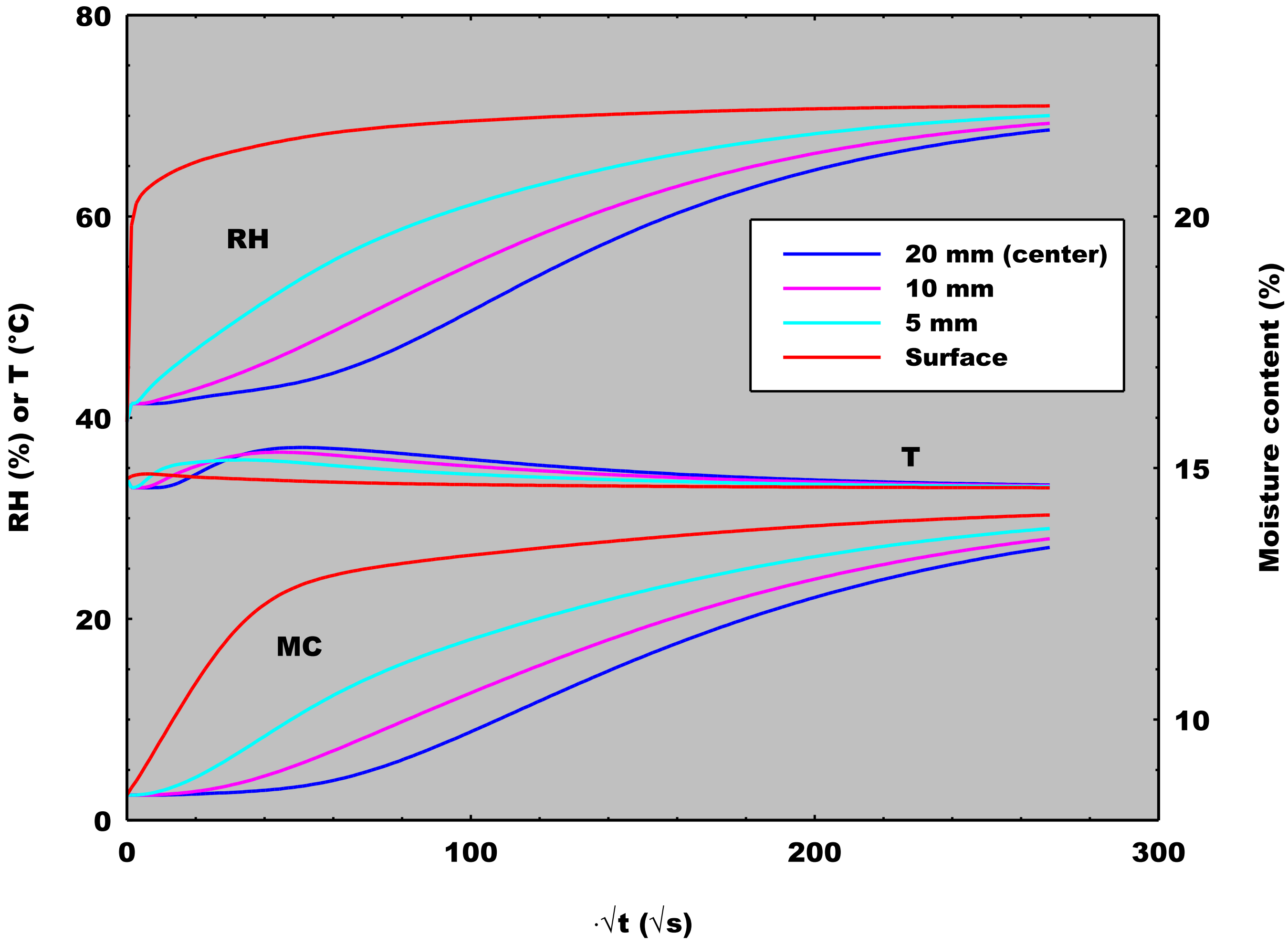


80
60
40
20
0
RH (%) or T (°C)
20
15
10
Moisture content (%)
0
100
200
300
·√t (√s)
RH
T
MC
20 mm (center)
10 mm
5 mm
Surface

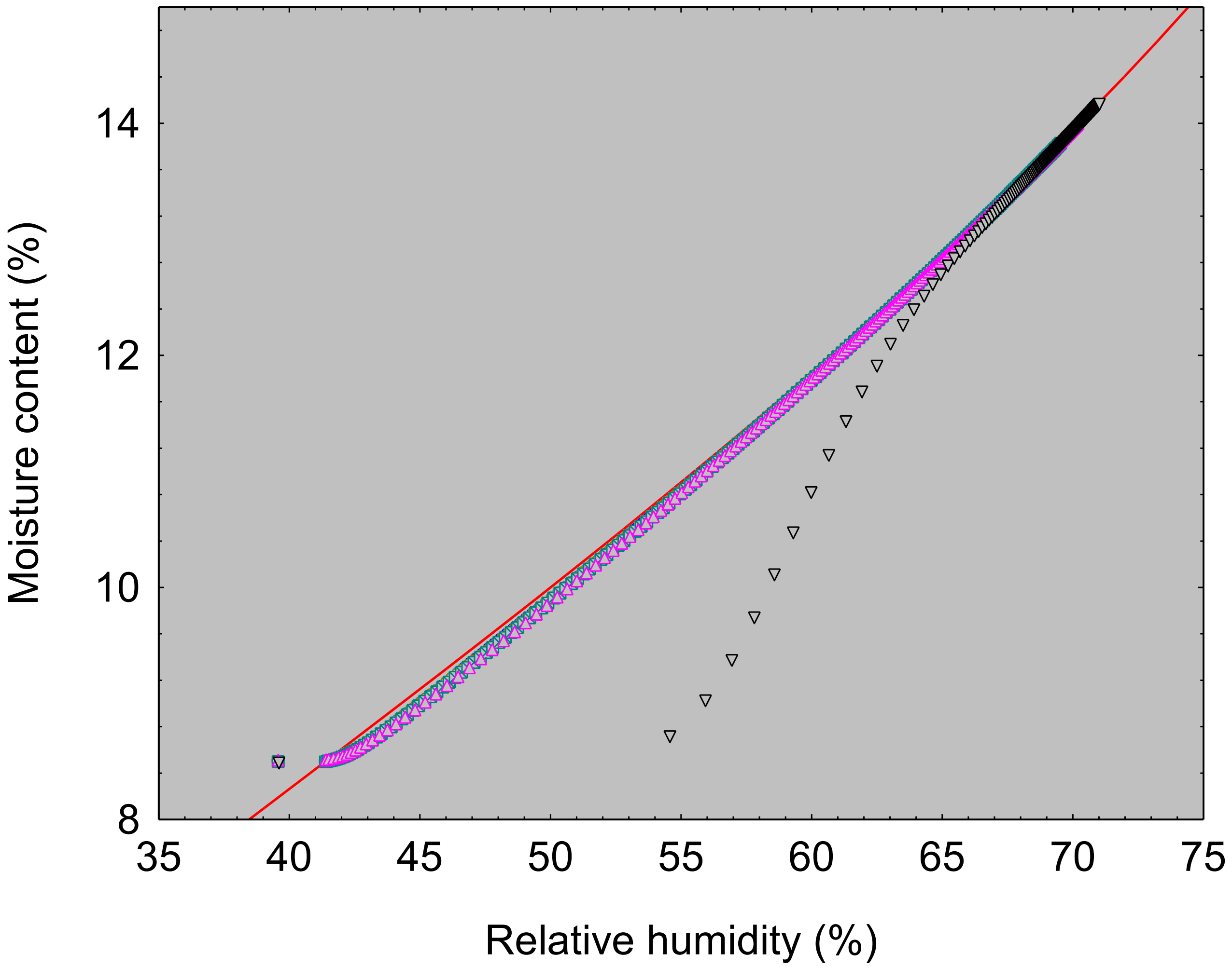
Test 2


80
60
40
20
0
0
100
200
300
20
15
10
RH (%) or T (°C)
Moisture content (%)
√t (√s)
RH
T
MC
20 mm (center)
10 mm
5 mm
Surface

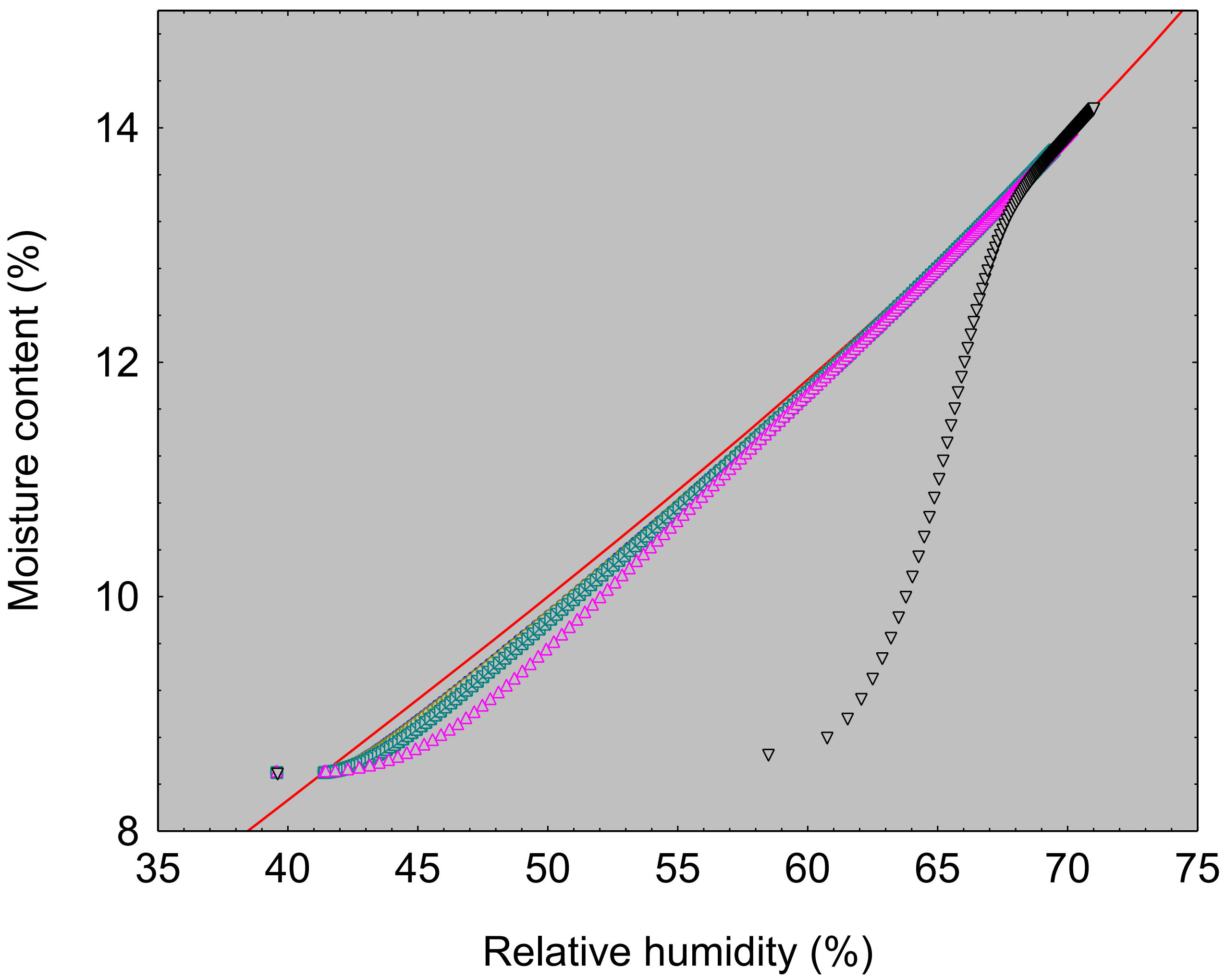
Test 3


80
60
40
20
0
RH (%) or T (°C)
0
100
200
300
·√t (√s)
20
15
10
Moisture content (%)
RH
T
MC
20 mm (center)
10 mm
5 mm
Surface

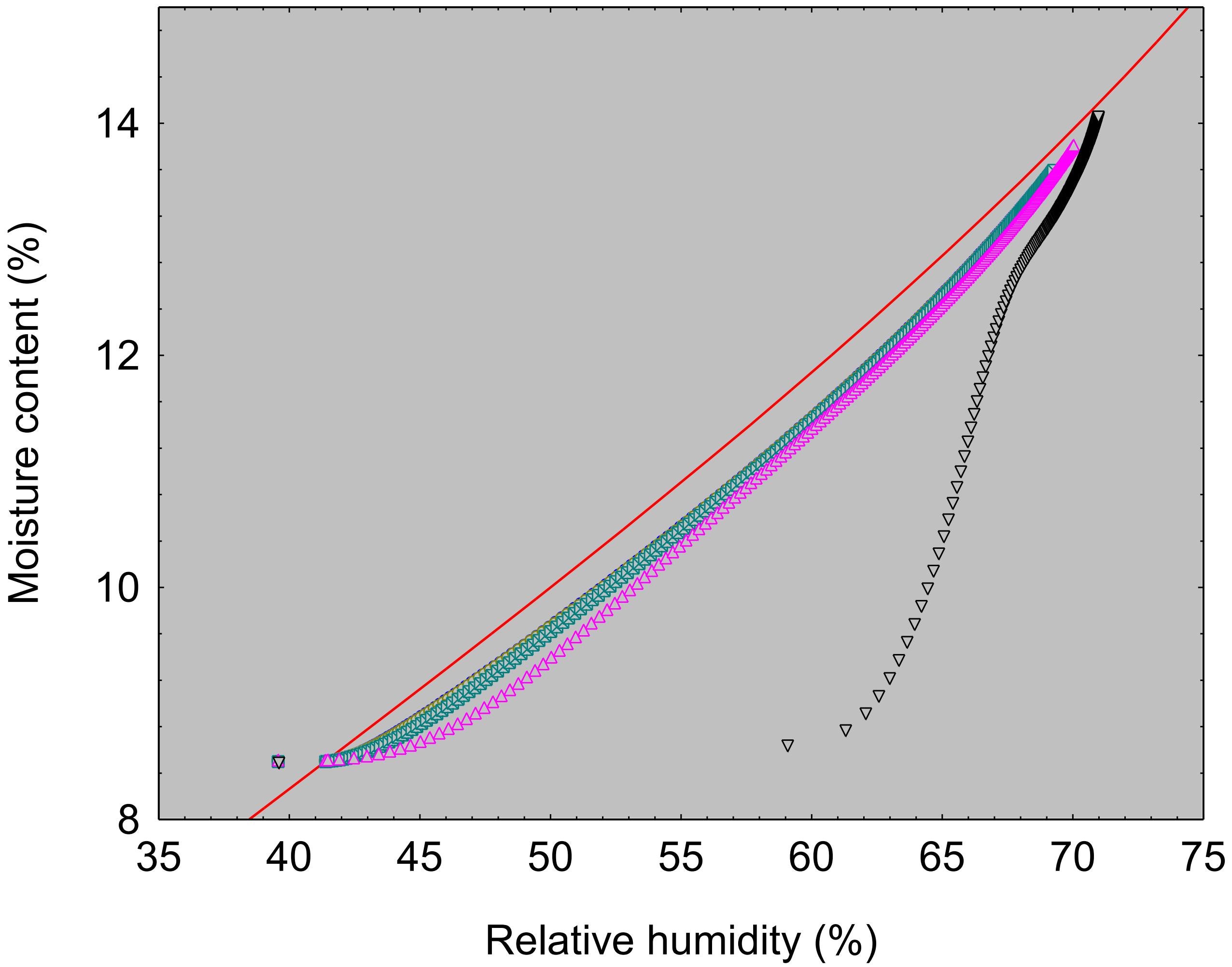
Test 1


Moisture content (%)
8
10
12
14
35
40
45
50
55
60
65
70
75
Relative humidity (%)

Test 2


Moisture content (%)
14
12
10
8
35
40
45
50
55
60
65
70
75
Relative humidity (%)

Test 3

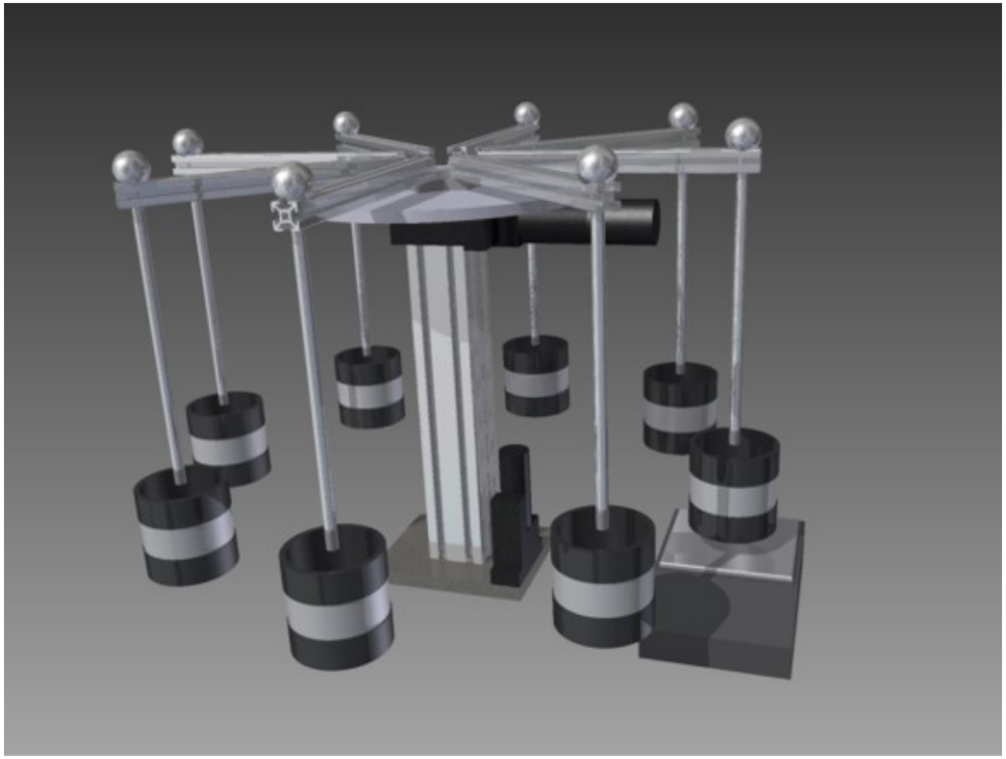

Moisture content (%)
14
12
10
8
35
40
45
50
55
60
65
70
75
Relative humidity (%)

The parallel flow model : quite simple but powerful:

- Sorption hysteresis
- Dual-scale effects
- Time delay due to macromolecular relaxation

One PhD work will start in September on this subject

A new specific device 'almost' in operation



+ BET and Rubotherm

X-ray µ-tomography
(ESRF, synchrontron beam, 0.7 µm spatial resolution)