AFCAT

jcat53 : JCAT53 - 53èmes Journées de Calorimétrie et d'Analyse Thermique

22-24 mai 2023 PALAISEAU (France)

Analyse thermique en présence de transferts couplés chaleur-masse : synergie entre expérimentation et modélisation

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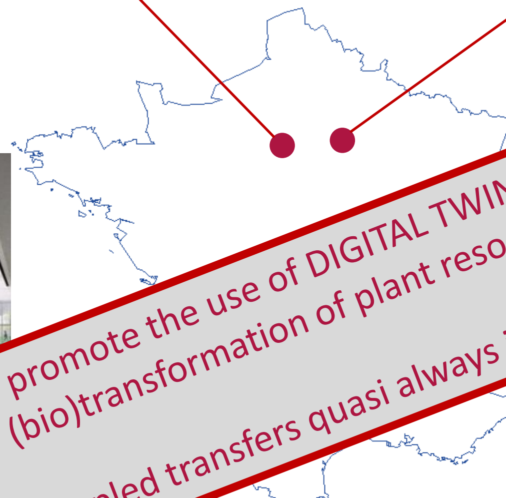
2nd top Engineering French "Grande Ecole"



We promote the use of DIGITAL TWIN in the (bio)transformation of plant resources

Coupled transfers quasi always involved

A group of 35+ at the CEBB, in the heart of the biorefinery of Bazancourt-Pomacle (nearby Reims)

Our supports

Marne LE DÉPARTEMENT

GRAND REIMS COMMUNAUTÉ URBAINE

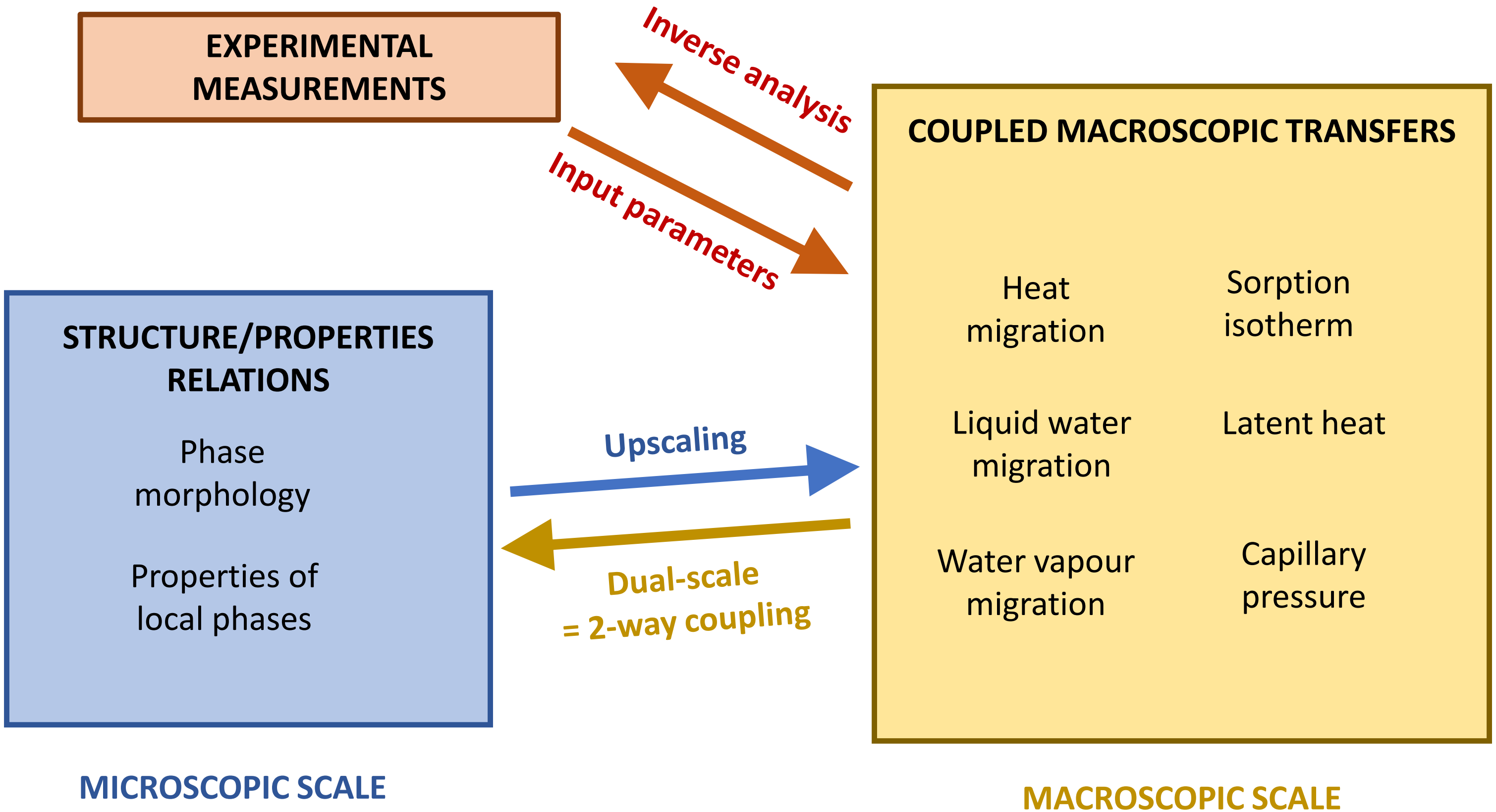
Grand Est ALSACE CHAMPAGNE-ARDENNE LORRAINE

UNION EUROPÉENNE Fonds Européen de Développement Régional

Vos 15 prochaines minutes

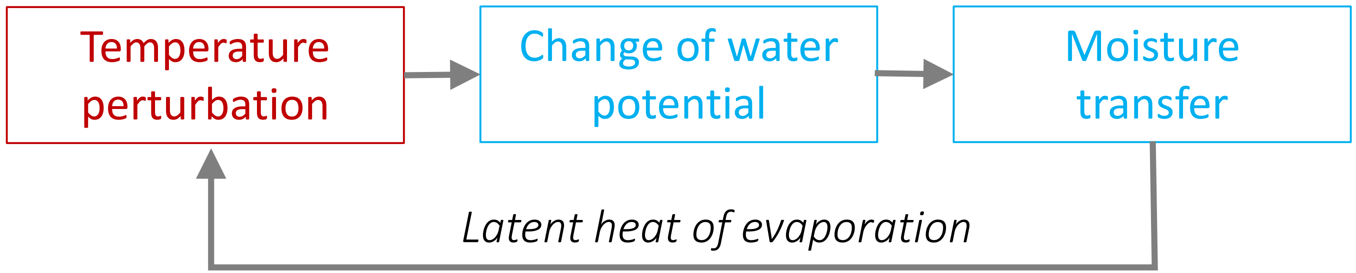
- Produits biosourcés = forte hygroscopicité
- Formulation/modélisation
- 3 exemples d’application en analyse thermique
- Conclusion

The physics of coupled transfers

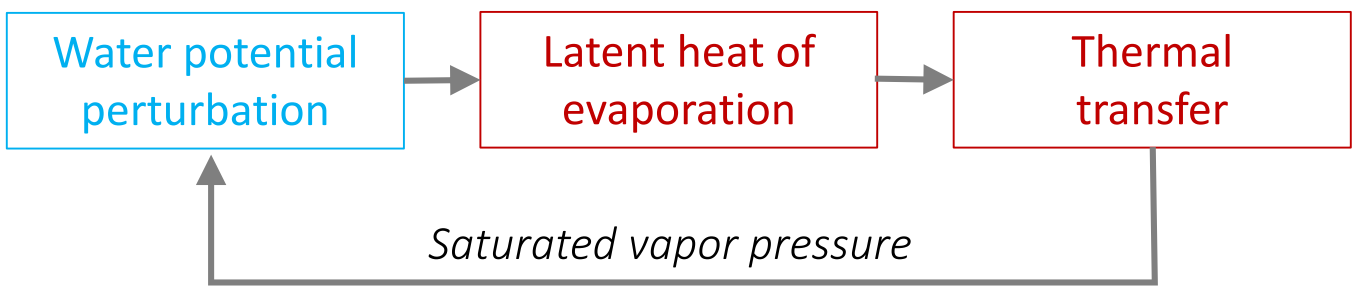


Characterisation of biosourced products

Thermal characterisation



Characterisation of moisture migration



The comprehensive macroscopic formulation

Moisture conservation

$$\rho_0 \frac{\partial X}{\partial t} + \nabla \cdot (\rho_w \bar{\boldsymbol{v}}_w + \rho_v \bar{\boldsymbol{v}}_g) = \nabla \cdot (\rho_g \boldsymbol{f} \boldsymbol{D}_v \nabla \omega_v + \rho_s \boldsymbol{D}_b \nabla X_b)$$

Energy conservation

$$\frac{\partial}{\partial t} \left(\varepsilon_w \rho_w h_w + \varepsilon_g (\rho_v h_v + \rho_a h_a) + \overline{\rho}_b \overline{h}_b + \varepsilon_s \rho_s h_s \right) + \nabla \cdot (\rho_w h_w \bar{\boldsymbol{v}}_w + (\rho_v h_v + \rho_a h_a) \bar{\boldsymbol{v}}_g) = \nabla \cdot (\lambda_{eff} \nabla T + \rho_g \boldsymbol{f} \boldsymbol{D}_v (h_v \nabla \omega_v + h_a \nabla \omega_a) + h_b \boldsymbol{D}_{b,\rho_v} \nabla \rho_v)$$

Air conservation

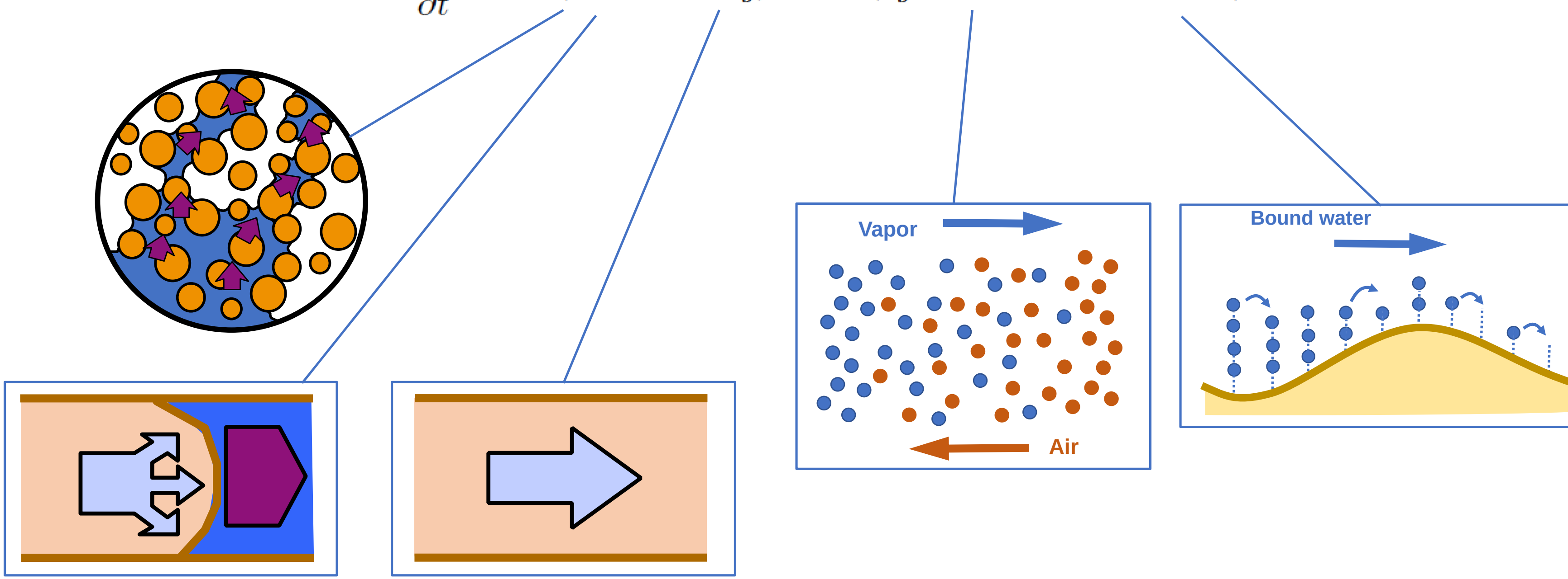
$$\frac{\partial \left(\varepsilon_g \rho_a \right)}{\partial t} + \nabla \cdot (\rho_a \bar{\boldsymbol{v}}_g) = \nabla \cdot (\rho_g \boldsymbol{f} \boldsymbol{D}_v \nabla \omega_a)$$

Perré, Turner (1999) Int. J. Heat Mass Transfer 42, 4501-4521.

The physics behind the macroscopic formulation

Moisture conservation

$$\rho_0 \frac{\partial X}{\partial t} + \nabla \cdot (\rho_w \bar{\boldsymbol{v}}_w + \rho_v \bar{\boldsymbol{v}}_g) = \nabla \cdot (\rho_g \boldsymbol{f} \boldsymbol{D}_v \nabla \omega_v + \rho_s \boldsymbol{D}_b \nabla X_b)$$



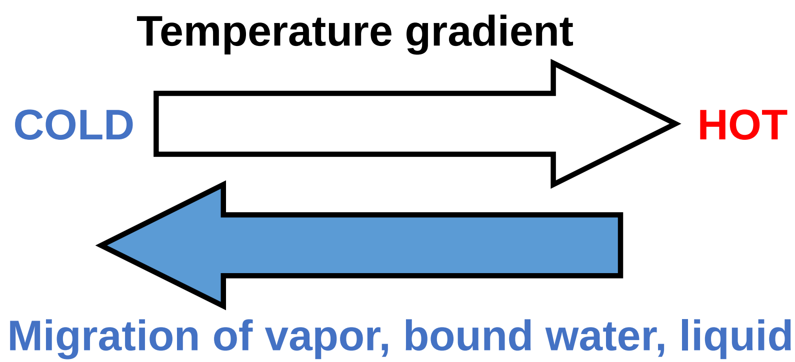
High temperature configurations

Perré et al., 2023 - State-of-the-art in the mechanistic modeling of the drying of solids: a review of 40 years of progress and perspectives, Drying Technology

The physics behind the macroscopic formulation

Thermo-migration

- Surface tension ↘ with temperature
- Pvs ↗ with temperature
- Thermo-activation



Perré et al., 2023 - State-of-the-art in the mechanistic modeling of the drying of solids: a review of 40 years of progress and perspectives, Drying Technology

Heat capacity measurement in the case of hygroscopic materials

Calvet Calorimeter C80

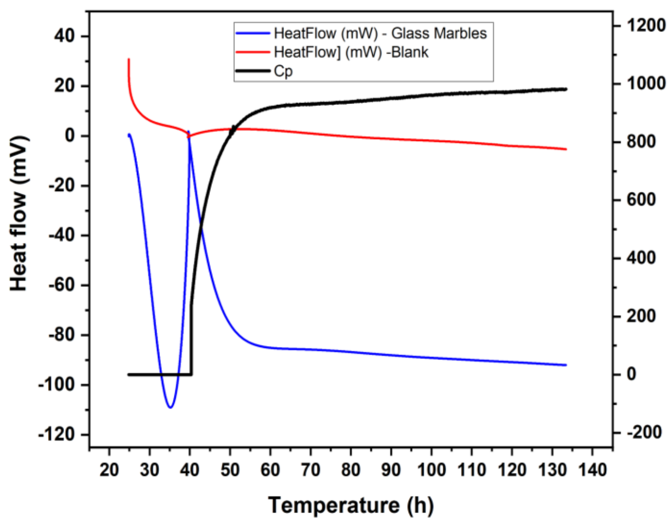
Batch cell

High Pressure cell

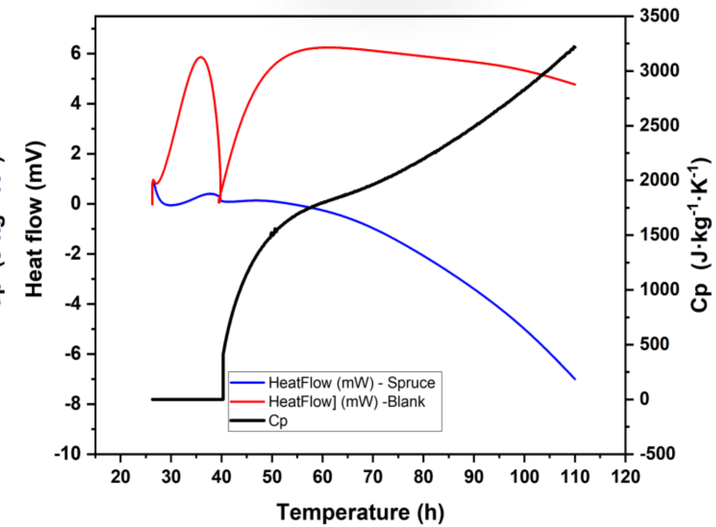
Wood sample

Batch cell

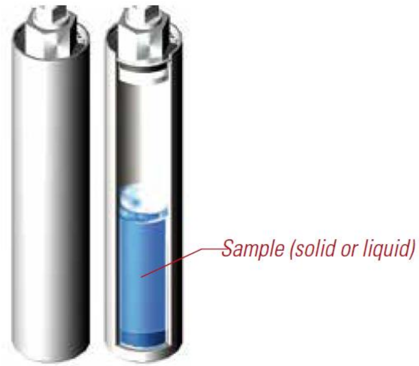
Inorganic materials
Glass beads



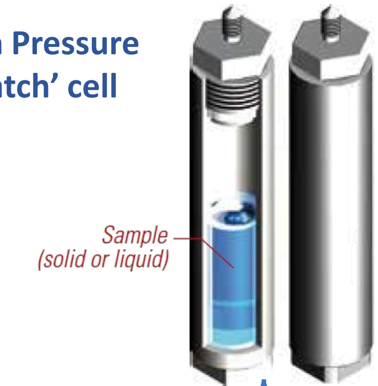
Wood
Spruce



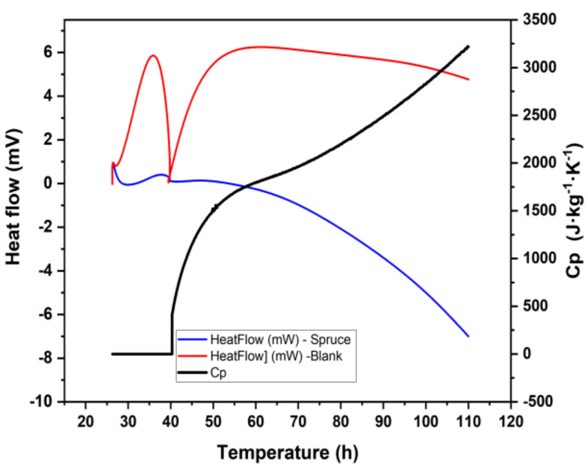
Batch cell



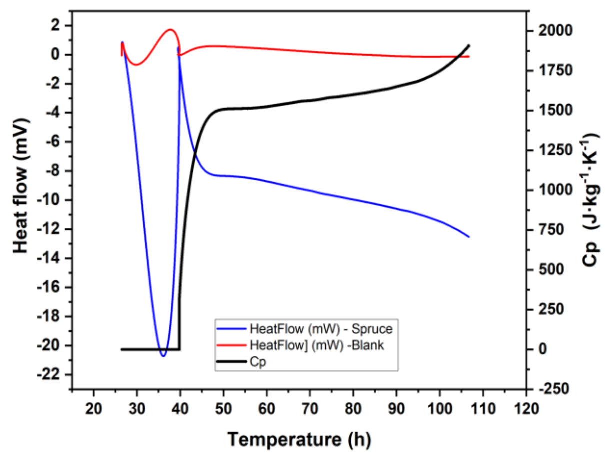
High Pressure 'Batch' cell



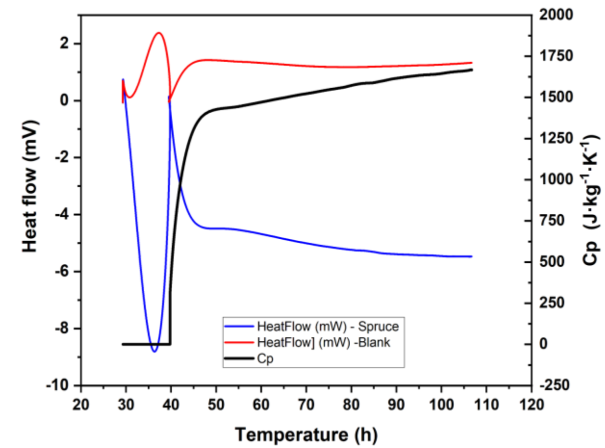
High Pressure cell is used when the sample evolves pressure, through a decomposition for example.



Without drying

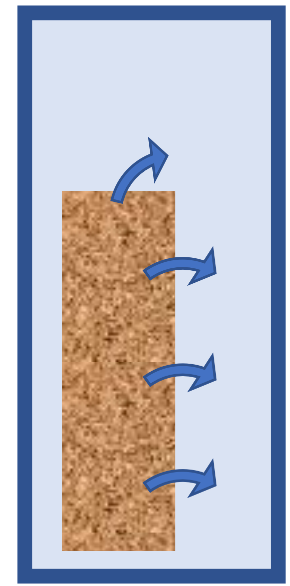


Dried samples at 105°C

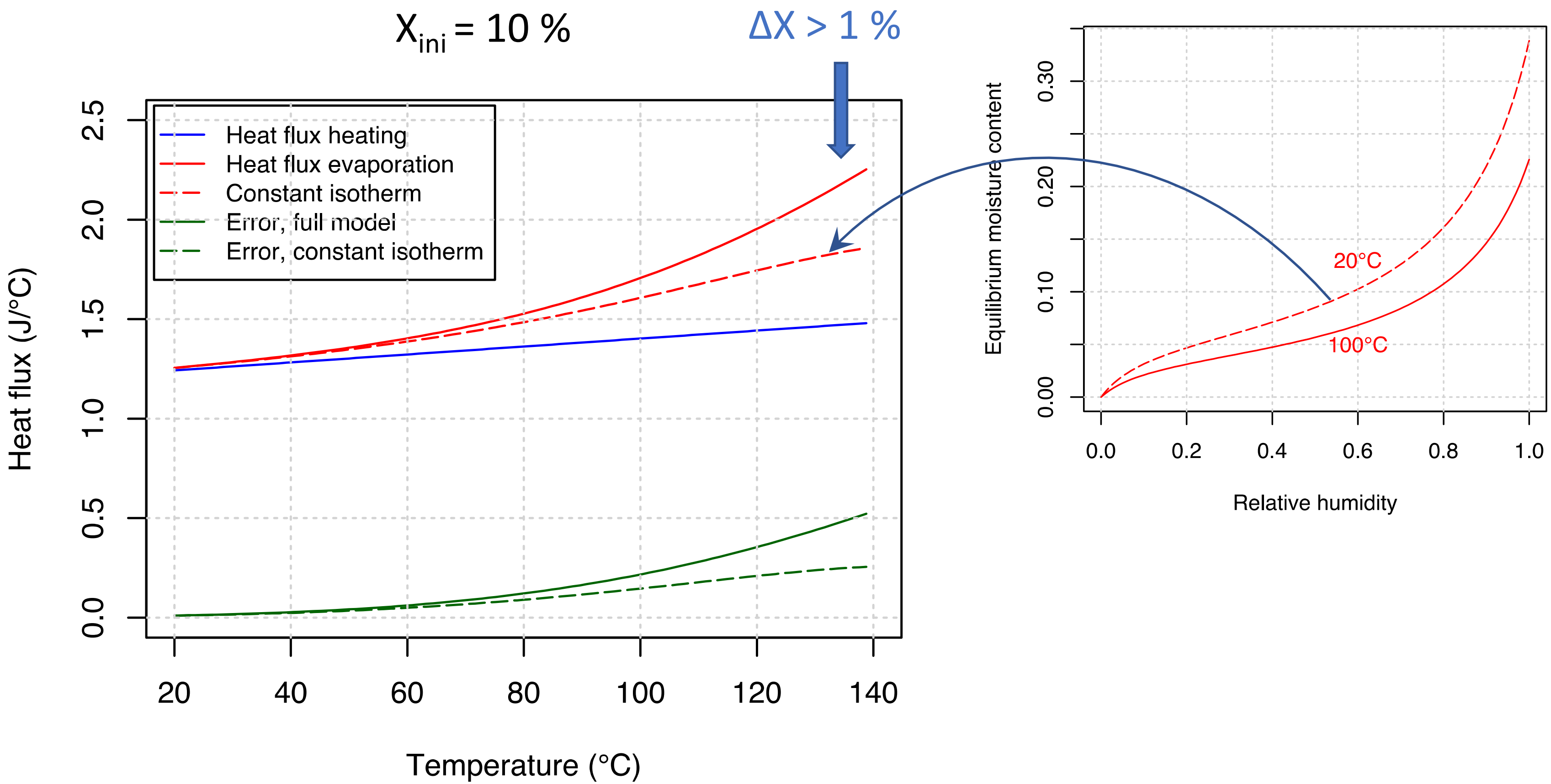


Simple simulation

- Sample mass and initial moisture content
- Crucible volume
- GAB sorption isotherm : X_{eq} = f(RH, T)
- Saturated water vapor pressure = f(T)
- Steady-state regime

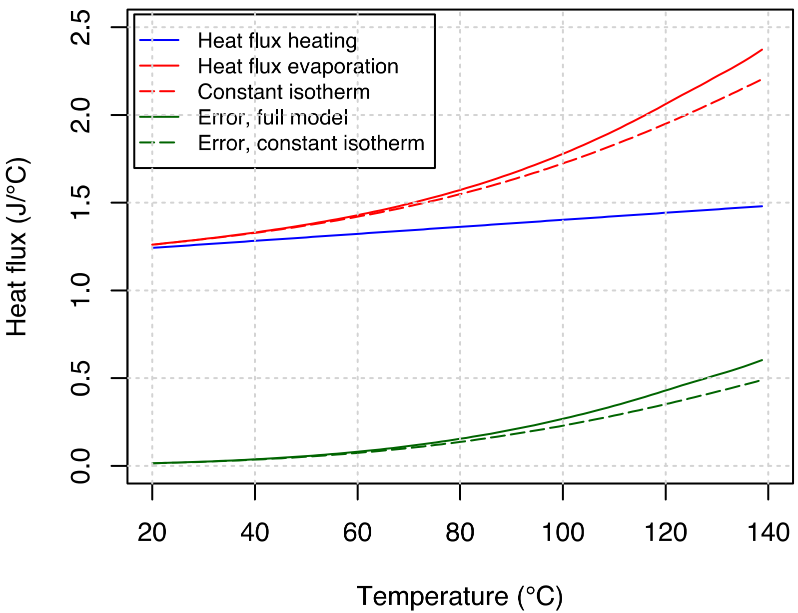


Simulation results

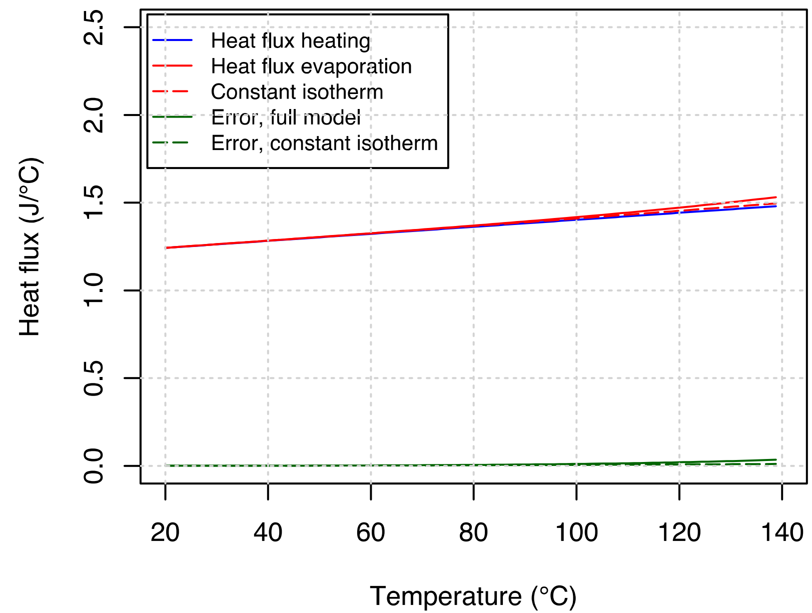


Simulation results

$X_{ini} = 20\ \%$



$X_{ini} = 1\ \%$



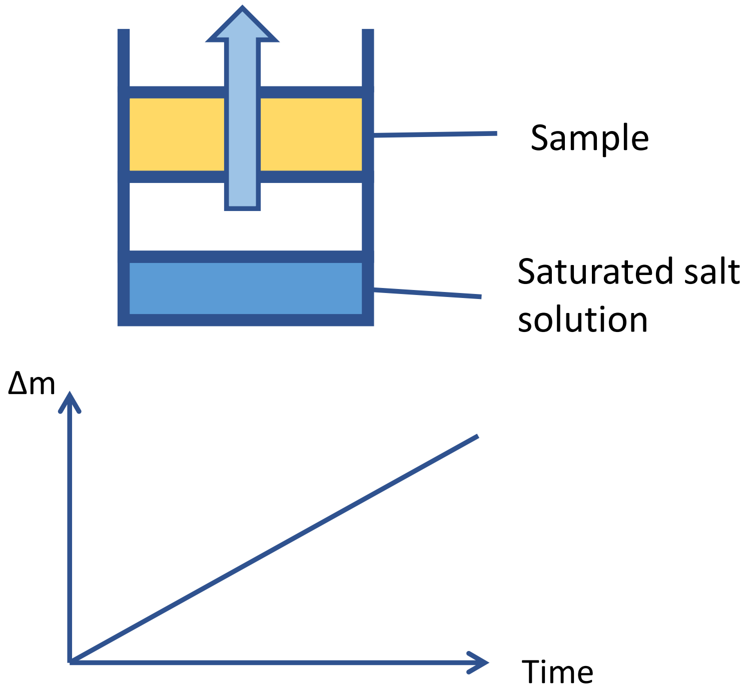
Recommendations

- Coupling negligible at low temperature (ca. 50°C)
- Mass to be increased to reduce the coupling (limitation of the heating rate)
- Coupling increase with moisture content (water activity)
- Good accuracy when sample oven-dry before the test.

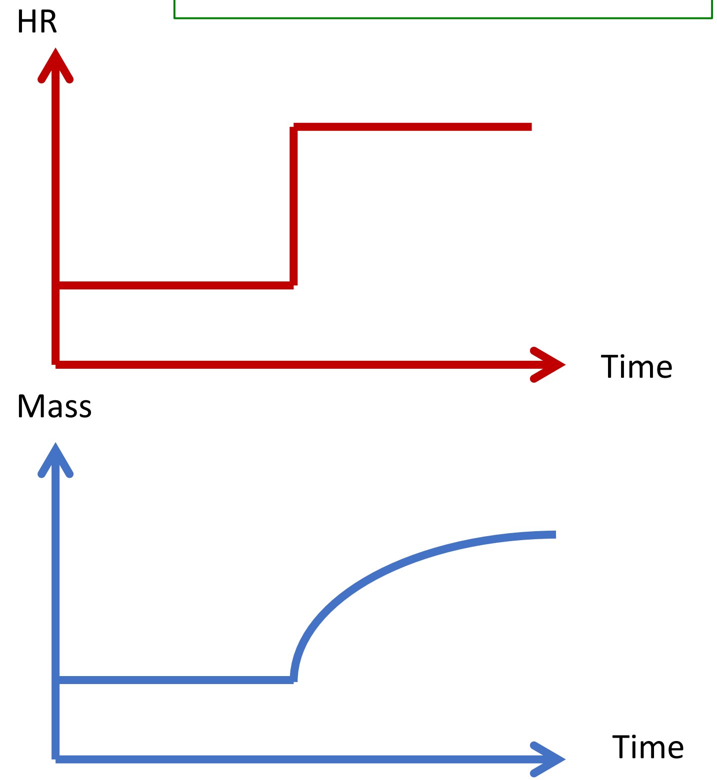
Mass diffusivity measurement

Classical methods

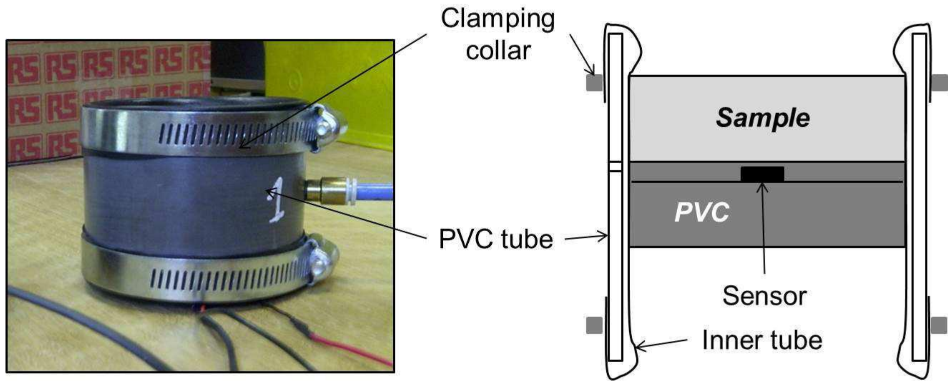
Cup method



Transient method



A new method : inverse analysis of the RH on the backside of the sample



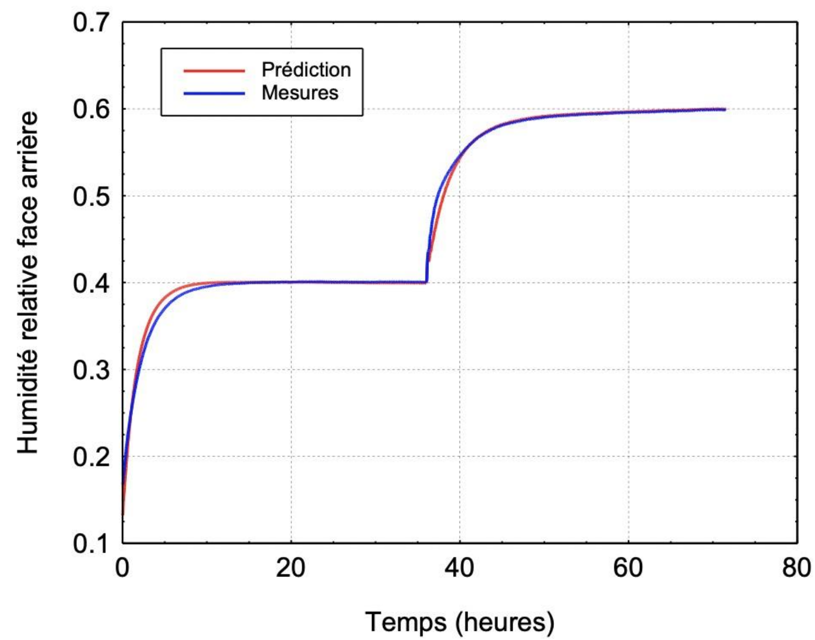
Principle

- The relative humidity varies on the exposed side and is simply measured on the back side (no need for perfect control)
- The mass diffusivity is determined by inverse method
- No moving pieces, several sample measured at the same time at low cost.

Requires a comprehensive physical model accounting for H&M coupling.

Perré, Pierre, Casalihno, Ayouz, Drying Technology, 2015

Back-face method :
mesure de la diffusivité à la vapeur d'eau

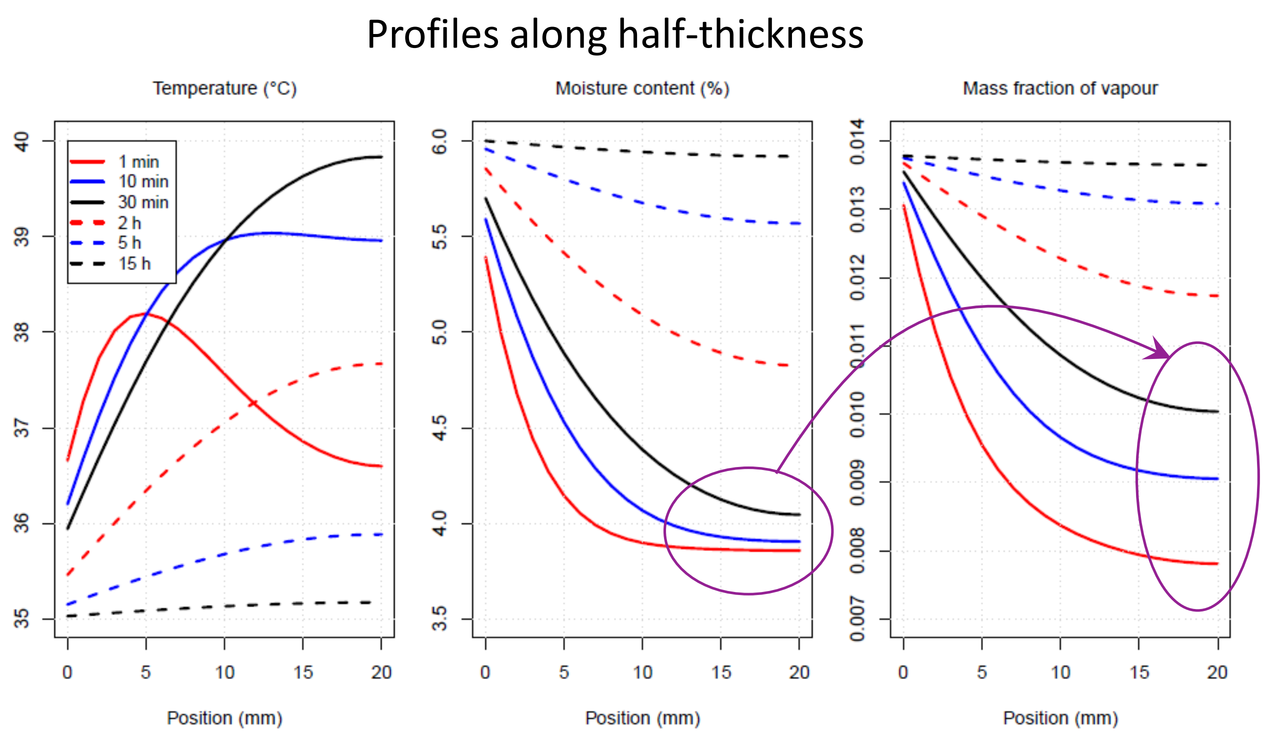


Perré P., Pierre F., Casalinho J., Ayouz M., Drying Technology, 2015

Some results

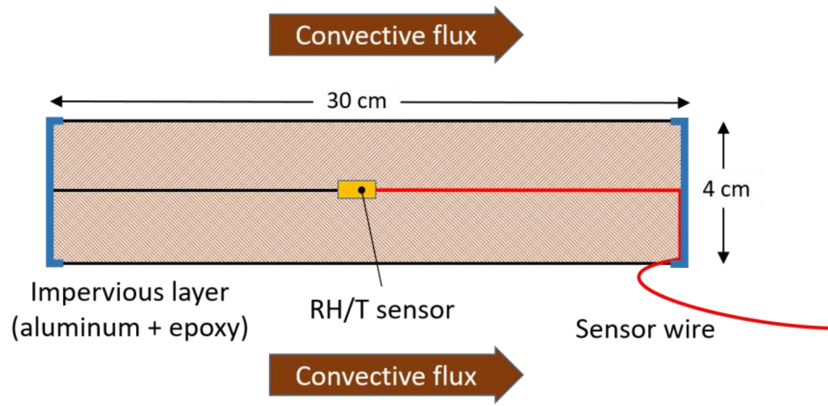
		f
MDF		0.285
Fiberboard		**>>1**
Spruce	Radial direction	0.024
	Tangential direction	0.017

Simulation results



Perré, Challansonnex, Colin (2019) Int. J. Heat Mass Transfer 133, 968-975.

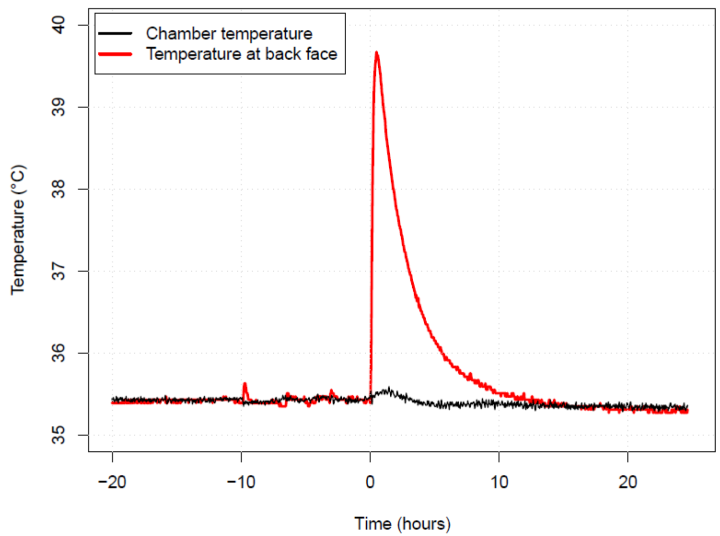
An specific experiment to obtain a symmetrical configuration

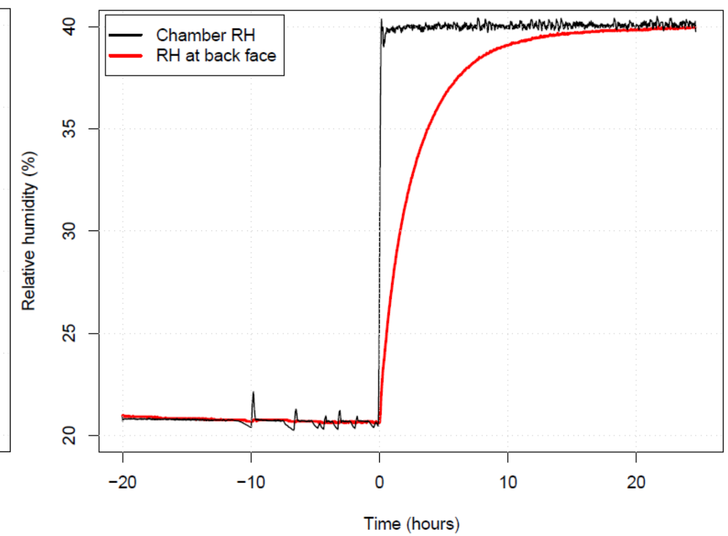


Sudden change to 40% RH after equilibrium at 20% RH

Perré, P. , Challansonnex, A., Colin, J. (2019), Int. J. Heat Mass Transfer 133, 968-975.

Experimental results



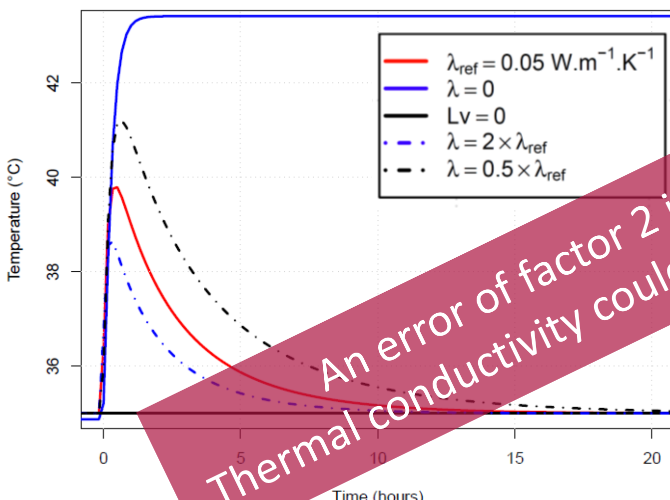


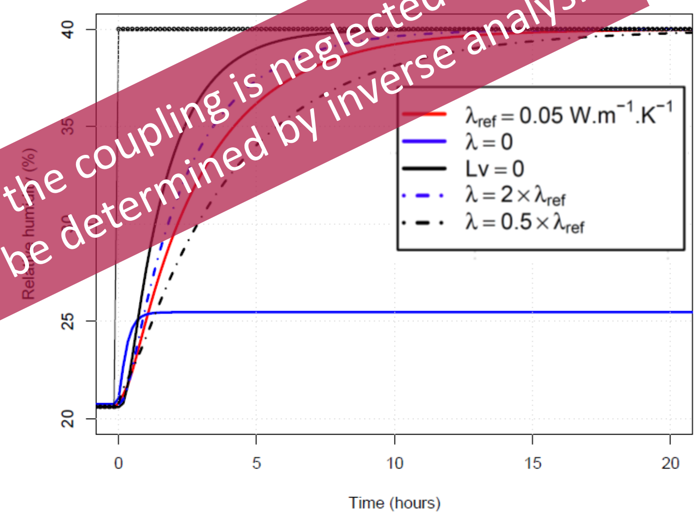
Impressive temperature peak in value (4°C) and duration (10 hours)

Perré, Challansonnex, Colin (2019) Int. J. Heat Mass Transfer 133, 968-975.

Changing thermal properties in the model

Red curves corresponds the identified diffusivity value



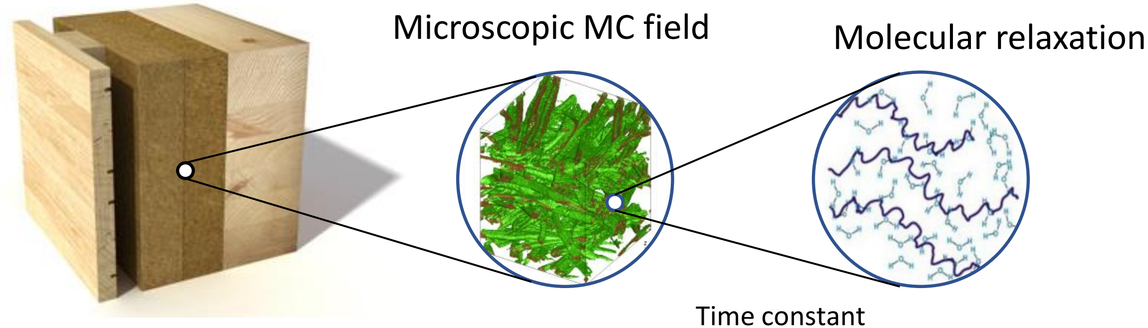


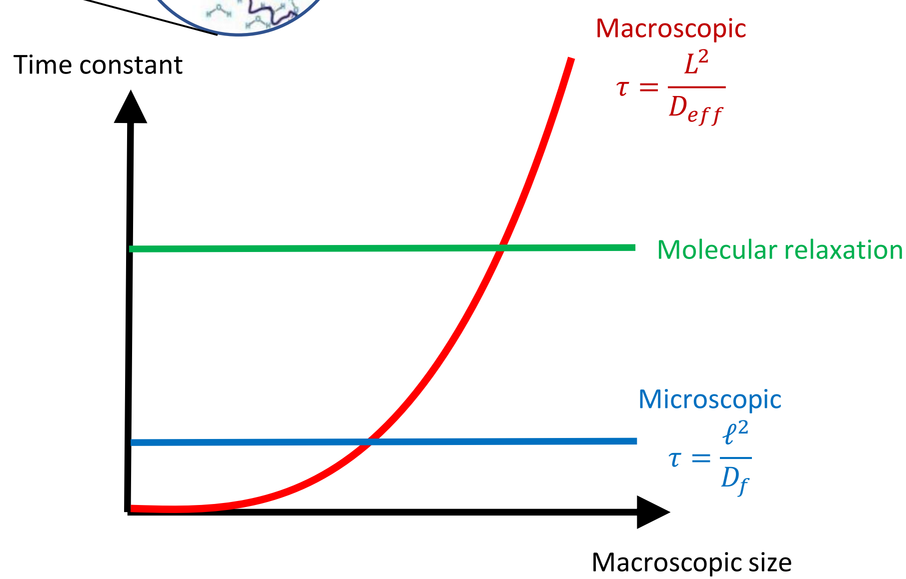
An error of factor 2 if the coupling is neglected
Thermal conductivity could be determined by inverse analysis

Perré, Challansonnex, Colin (2019) Int. J. Heat Mass Transfer 133, 968-975.

Failure of local equilibrium : multiscale effects

Three intricate spatial scales

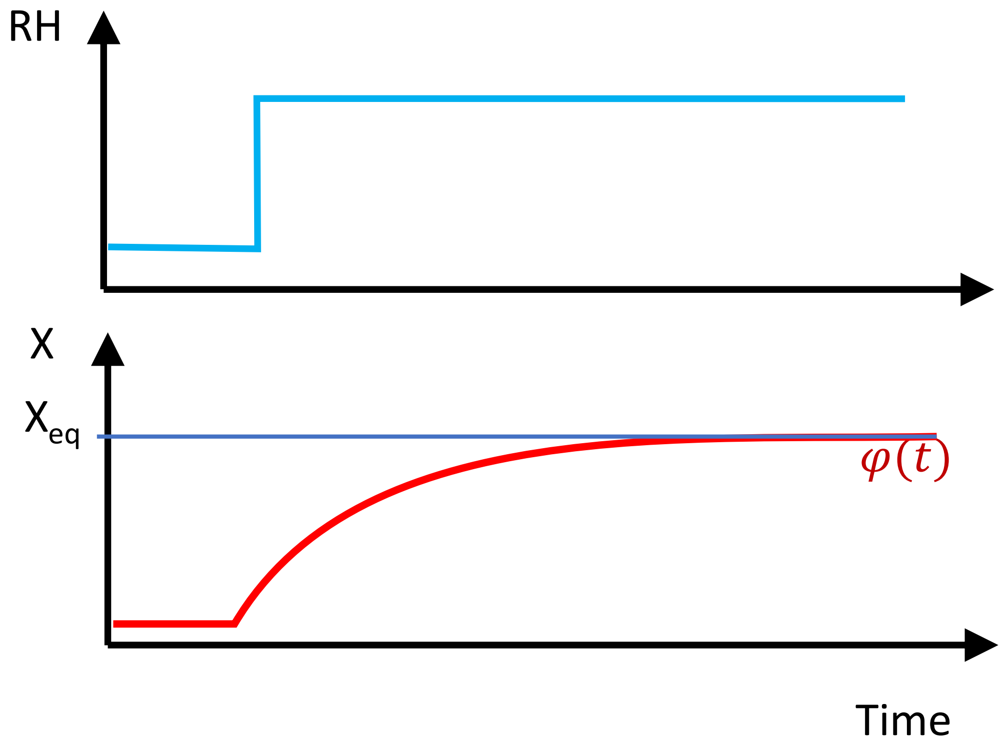




P. Perré (2019), Int. J. Heat Mass Transfer, 140: 717–730

Macroscopic formulation : memory function

Local behaviour following a sudden change in RH



$$X(t) - X_{ini} = \Delta X_{eq} \times \varphi(t)$$

Where φ is the memory function

Macroscopic formulation : memory function

The modified heat & mass transfer model

Moisture conservation

$$\frac{\partial}{\partial t}\left(aX_{eq} + \int_0^t k(t-\tau)X_{eq}d\tau\right) = \nabla \cdot (\boldsymbol{D}_b \nabla X_{eq}) \qquad (15)$$

Energy conservation

$$\frac{\partial}{\partial t}\left(\rho_b \overline{h}_b + \varepsilon_s \rho_s h_s\right) = \nabla \cdot (\lambda_{eff} \nabla T + h_b \rho_s \boldsymbol{D}_b \nabla X_{eq}) \qquad (16)$$

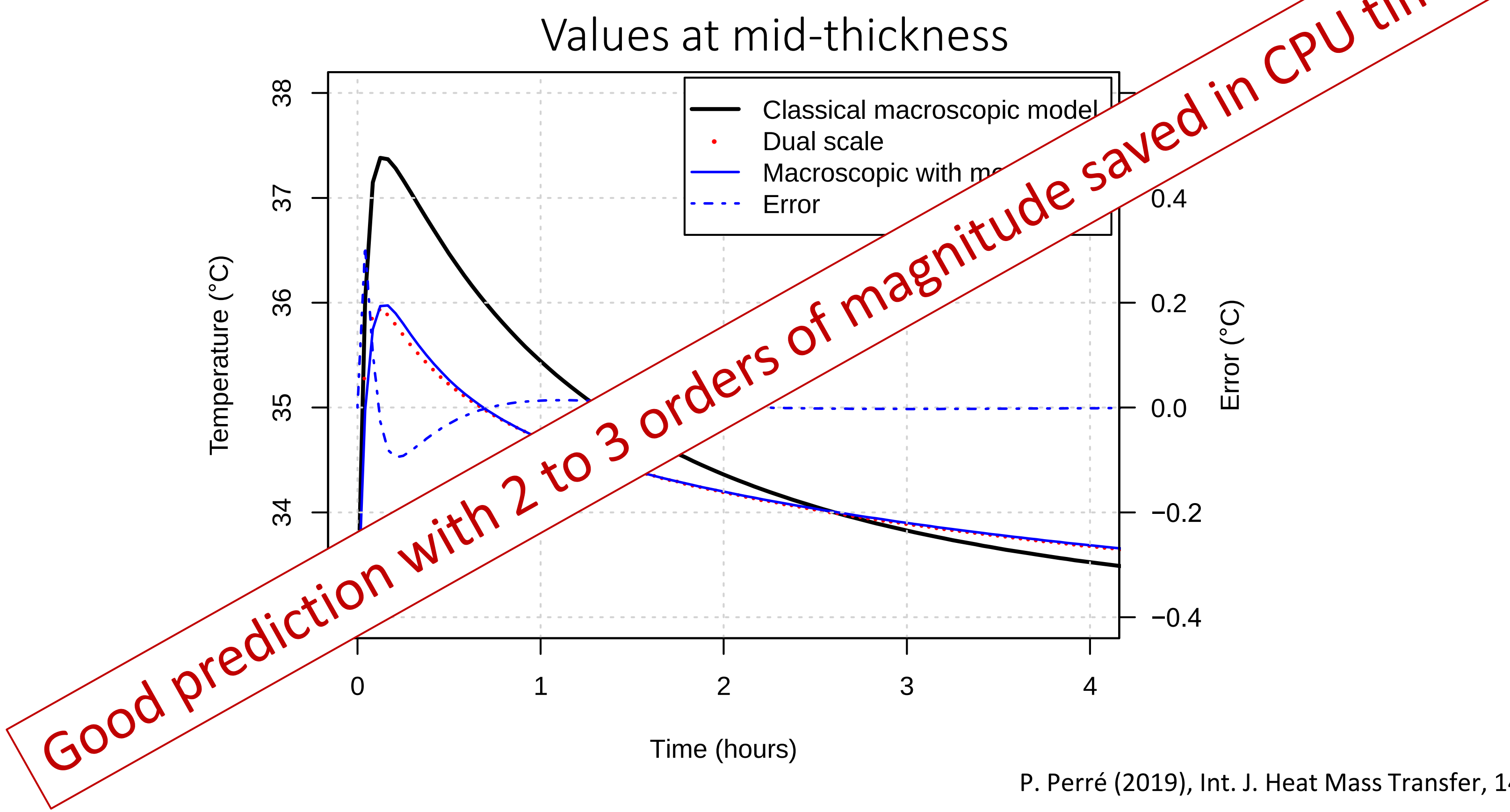
Non-local equilibrium

$$X(t) = X_{eq}(t) - \sum_i \phi_i(t) \qquad (17)$$

One internal variable per exponential function

P. Perré (2019), Int. J. Heat Mass Transfer, 140: 717–730

Validation : temperature



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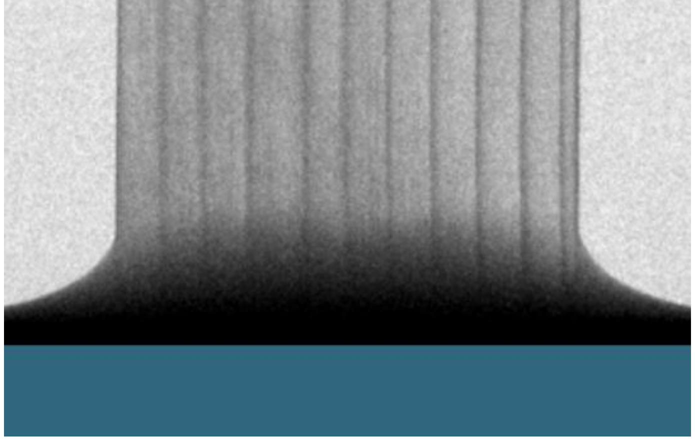

Thank you for your attention !