Novel approaches to multiscale modelling in bio-based materials

Talk title: A novel analytical model for predicting the effective thermal conductivity tensor of lime-hemp concrete and hemp insulation

Anh Dung Tran Le

Laboratoire des Technologies Innovantes, EA 3899

Université de Picardie Jules Verne, Amiens France

anh.dung.tran.le@u-picardie.fr

Septembre 2022

UNIVERSITÉ de Picardie Jules Verne

Contents lists available at ScienceDirect

Energy & Buildings

journal homepage: www.elsevier.com/locate/enbuild

A novel anisotropic analytical model for effective thermal conductivity tensor of dry lime-hemp concrete with preferred spatial distributions

Anh Dung Tran-Le[a,*], Sy-Tuan Nguyen[b], Thierry Langlet[a]

PLAN

- **Contexte et généralités**
- **Propriétés microscopiques**
- **Méthode d'homogénéisation**
- **Validation**
- **Application**
- **Conclusion**

Goal for building design

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

Hygrothermal comfort → 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*

Bio-based materials

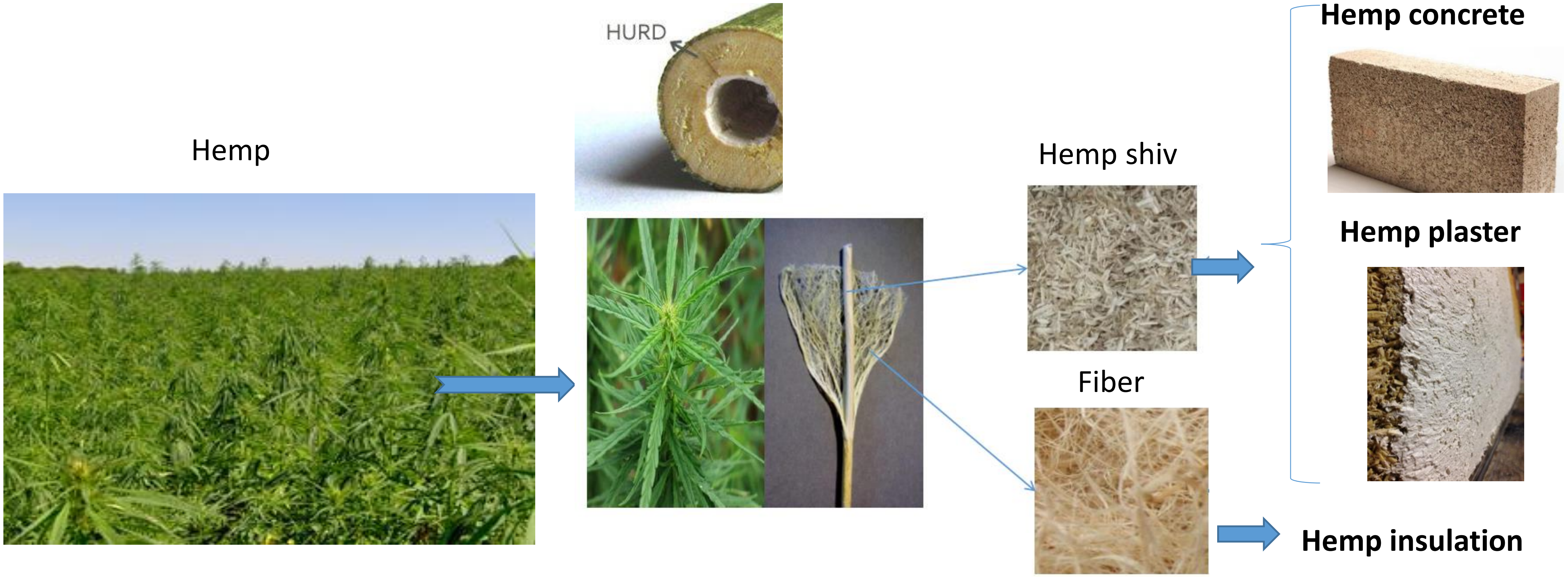
Colza
Disponibilité nationale (France)

Lin
Disponibilité régionale (Hauts-de-France)

Chanvre (matériau considéré comme référence)
Disponibilité nationale (France)

France qui est le premier pays producteur européen.

Valorization of Hemp in building construction



Components of hemp concrete

Chènevotte

\+

1/3 Chaux hydraulique
\+
2/3 chaux aérienne

\+

Eau

Manufacturing process of hemp concrete

Mélange 1

Chaux : Tradical PF70

\+ Eau

\+

Mélange 2

Chènevotte

\+ Eau

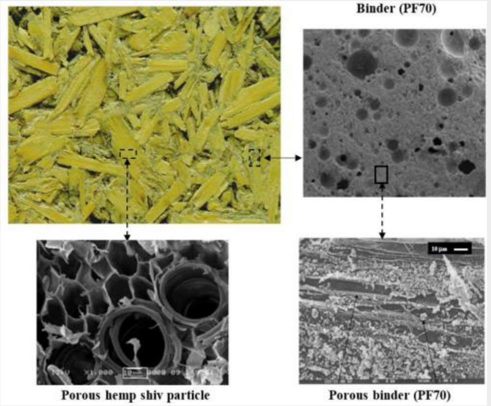
=

Béton de chanvre classique

Novel approaches to multiscale modelling in bio-based materials: the case of lime hemp concrete

Démarche multi-échelle (micro au local)

Échelle microscopique



Propriétés microscopiques des composantes

Échelle du matériau

Propriétés
- Thermique
- Physique
- Hygrique

Échelle de la paroi

Comportement hygrothermique

Étude expérimentale et **validation**

Échelle du local

Simulation du comportement hygrothermique pour prédire la QAI, le confort et consommation

Méthode d'homogénéisation
Et validation

Intégration des données

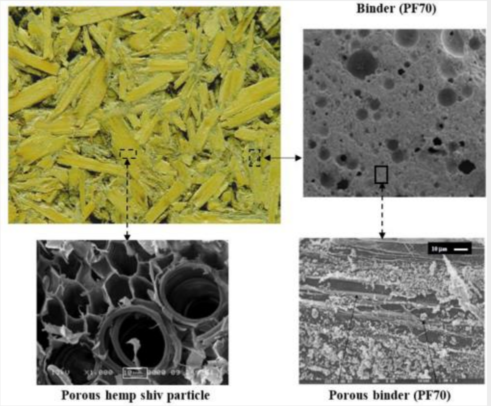
Modèle complet HAM* paroi

Modèle complet HAM* local

***HAM**: Combined Heat, air and moisture transport model

Démarche multi-échelle (microscopique au local)

Échelle microscopique



Propriétés microscopiques des composantes

Échelle du matériau

Propriétés
Thermique
Physique
Hygrique

It is the « Talk title »

Modèle complet HAM* paroi

Modèle complet HAM* local

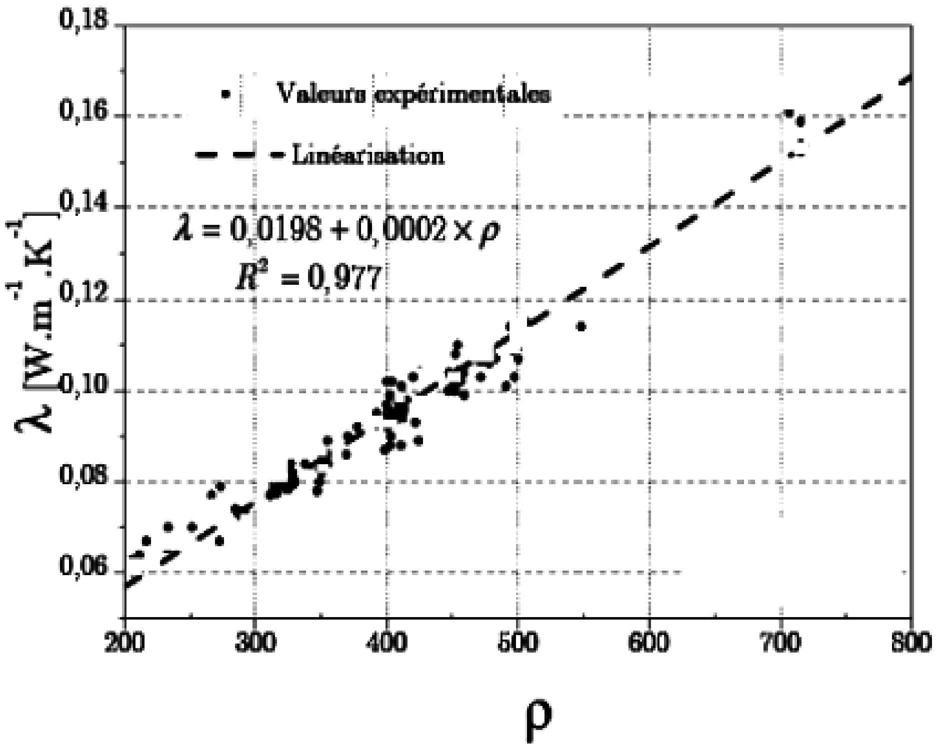
Méthode d'homogénéisation

Intégration des données

***HAM**: Combined Heat, air and moisture transport model

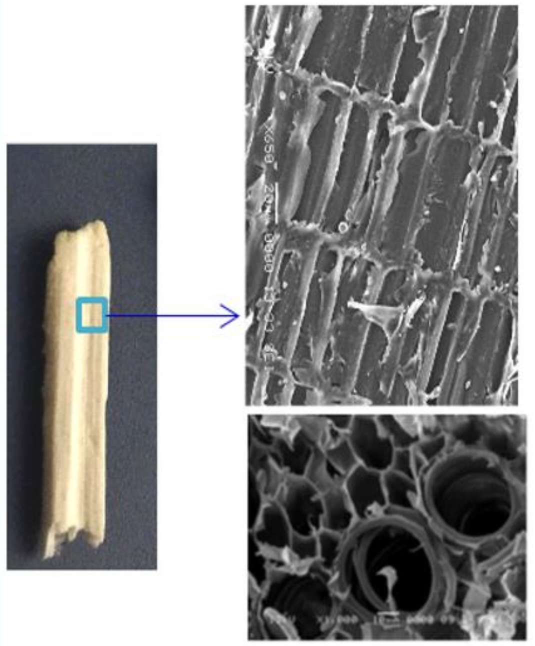
A novel analytical model for predicting the effective thermal conductivity tensor of lime-hemp concrete (LHC)

- Thermal conductivity of hemp concrete can be *directly measured in laboratory*.
- Up to date, the thermal con- ductivity of LHC is generally expressed *as a scalar*.
- Hemp concrete is generally either cast or sprayed, its thermal conductivity is direction dependent: *the arrangements of hemp particles are different in different directions*.

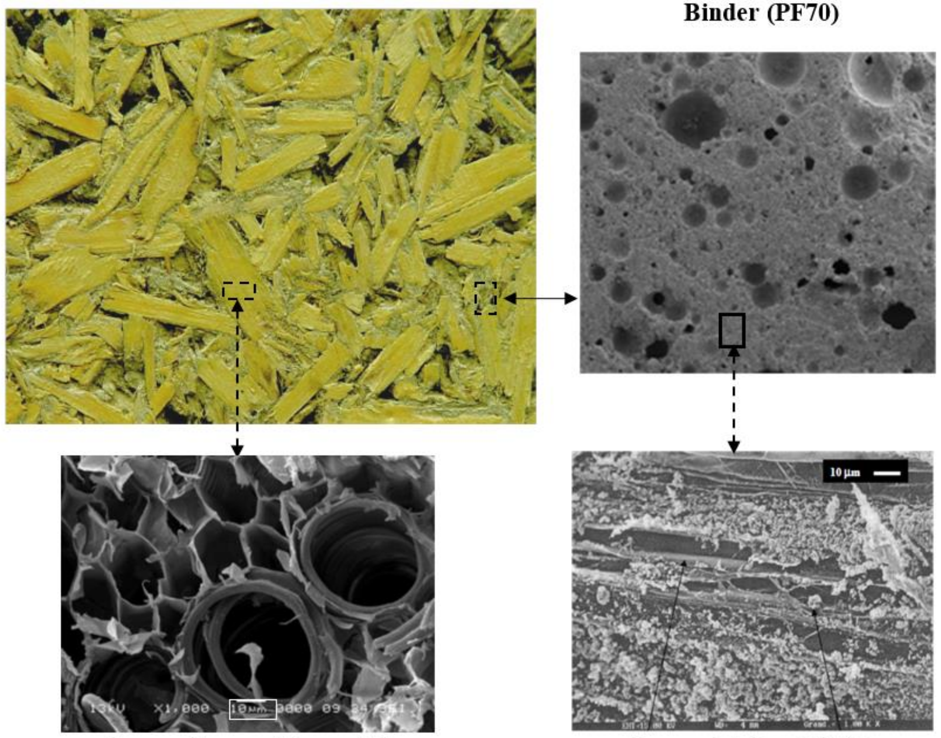


La conductivité thermique du béton de chanvre sec en fonction de la masse volumique (Cerezo, 2008).

Microscopy of hemp shiv and binder


3D real hemp shiv particle and its microstructure, morphology

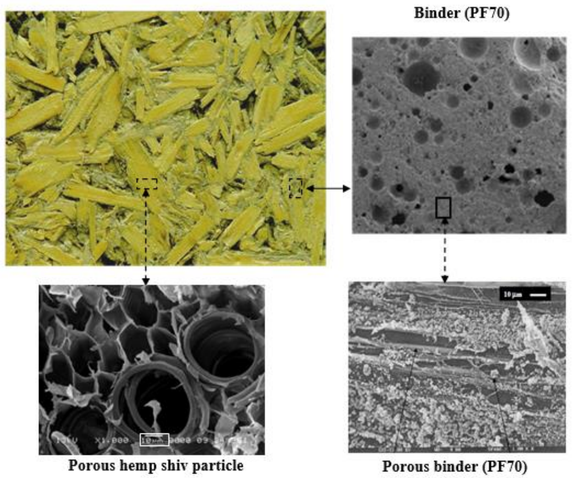
Hemp shiv

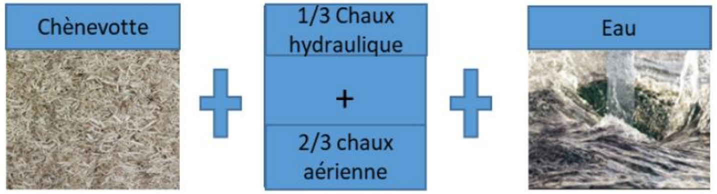


Porous hemp shiv particle
Porous binder (PF70)

Hemp concete

A novel analytical model for predicting the effective thermal conductivity tensor of lime-hemp concrete





Developed model takes into account:

- Hemp shiv particles
- Binder type
- Formulation of hemp concrete
- Manufacturing process
- Durability and surface treatment

Predicted thermal properties of hemp concrete

Nomenclature

Notations	Physical meanings	Units
λ	Thermal conductivity	$W/(m.K)$
$\boldsymbol{\lambda}$	Thermal conductivity tensor	$W/(m.K)$
X	Aspect ratio of the inclusion	–
ν, Q	Anisotropic parameters of the inclusion	–
α	Interface parameter	–
f	Volume fraction of a phase	–
φ	Porosity	–
ρ	Density	kg/m^3
$\boldsymbol{\delta}$	Kronecker delta	–
$\boldsymbol{A}$	Second order localization tensor	–
$\boldsymbol{P}$	Second order Hill's tensor	$m.K/W$
n	Number of phases in a composite material	–
$\underline{e}_3$	Unit vector in the axial direction of a spheroidal inclusion	–
m	Distribution parameter	–
W	Distribution function	–
Γ	Root mean square difference of the thermal conductivity	$W/(m.K)$

Basis formulations of the homogenization method

The overall conductivity of a heterogeneous medium can be obtained by considering the relationship between the local and the macroscopic behavior of a Representative Elementary Volume (REV)

$$\underline{q}(\underline{z}) = -\boldsymbol{\lambda}(\underline{z})\underline{\nabla T}(\underline{z}) \quad (1)$$

$$\underline{Q} = -\boldsymbol{\lambda}^{hom}\underline{\mathbf{E}} \quad (2)$$

$$\underline{Q} = \frac{1}{|\Omega|}\int_{\Omega} \underline{q}(\underline{z})d\Omega \quad (3)$$

$$\underline{E} = \frac{1}{|\Omega|}\int_{\Omega} \underline{\nabla T}(\underline{z})d\Omega \quad (4)$$

where $\underline{q}(\underline{z})$, $\underline{\nabla T}(\underline{z})$ and $\boldsymbol{\lambda}(\underline{z})$ are the local heat flux vector, the local thermal gradient field and the local conductivity tensor at a point $\underline{z}$ inside the REV, respectively;

$\underline{Q}$, $\underline{\mathrm{E}}$ and $\boldsymbol{\lambda}^{hom}$ are the overall heat flux vector, thermal gradient field and conductivity tensor of the REV, respectively; $|\Omega|$ the volume of the REV

Basis formulations of the homogenization method

The local and the average thermal gradient field tensors are related by the following linear equation:

$$\underline{\nabla T}(\underline{z}) = \boldsymbol{A}(\underline{z})\underline{\mathrm{E}} \qquad (5)$$

The combination of equations (1) to (5) yields the following equation to calculate the overall conductivity tensor of the REV:

$$\boldsymbol{\lambda}^{hom} = \frac{1}{|\Omega|}\int_{\boldsymbol{\Omega}} \boldsymbol{\lambda}(\underline{z})\boldsymbol{A}(\underline{z})d\Omega \qquad (6)$$

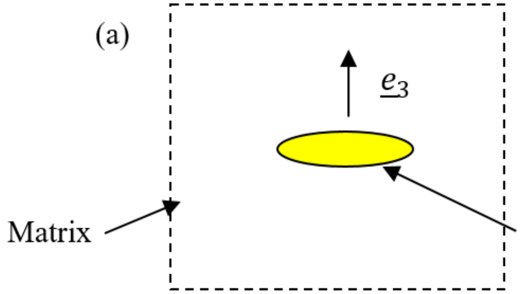
In equation (6),

- the local ***conductivity tensor*** $\boldsymbol{\lambda}(\underline{z})$ is assumed ***to be known***
- the main question is to determine the ***localization tensor*** $\boldsymbol{A}(\underline{z})$.

Basis formulations of the homogenization method

The extension of the Eshelby's solution (Eshelby, 1957) (single *ellipsoidal inclusion* in *an infinite homogeneous matrix* (Figure 1 a), for *transport property*) provides an analytical solution of $\boldsymbol{A}$, noted by $\boldsymbol{A}^*$

$$\boldsymbol{A}^* = \left(\boldsymbol{I} + \boldsymbol{P}(\boldsymbol{\lambda}_{inc} - \boldsymbol{\lambda}_m)\right)^{-1} \qquad (7)$$



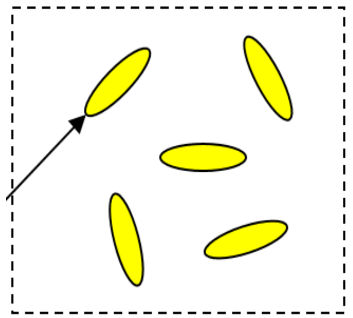
$\boldsymbol{\lambda}_{inc}$ and $\boldsymbol{\lambda}_m$ are the conductivity tensors of the inclusion and of the matrix reference,

$\boldsymbol{I}$ the second order unit tensor.

The second order tensor $\boldsymbol{P}$ is the Hill tensor (Hill, 1965), that depends both on the shape of the inclusion and the conductivity of the reference matrix.

For the general case of **multi-inclusions** (Figure 1 b), (***Dormieux et al., 2006***)

$$\boldsymbol{A} = \boldsymbol{A}^* \overline{\boldsymbol{A}^*}^{-1} \qquad (8)$$



$\overline{a}$: average over the whole domain of a value a: $\overline{a} = \frac{1}{|\Omega|}\int_{\Omega} a d\Omega$.

Basis formulations of the homogenization method

The combination of equations (6) to (8) yields:

$$\boldsymbol{\lambda}^{hom} = \overline{\boldsymbol{\lambda}(\boldsymbol{I} + \boldsymbol{P}(\boldsymbol{\lambda} - \boldsymbol{\lambda}_m))^{-1}}\,\overline{\left(\boldsymbol{I} + \boldsymbol{P}(\boldsymbol{\lambda} - \boldsymbol{\lambda}_m)\right)^{-1}}^{-1} \quad (9)$$

Equation (9) can be expressed by following well-known formula

$$\boldsymbol{\lambda}_{hom} = \left(\sum_{i=1}^{n} f_i \boldsymbol{\lambda}_i \boldsymbol{A}_i\right)\left(\sum_{i=1}^{n} f_i \boldsymbol{A}_i\right)^{-1} \quad (10)$$

n is the number of the inhomogeneities;

f_i and $\boldsymbol{\lambda}_i$ the volume fraction and the thermal conductivity of an inhomogeneity i, respectively;

$\boldsymbol{A}_i$ the localization tensor that is function of the conductivity and shape of the phase i and the conductivity of the surrounding matrix

Basis formulations of the homogenization method

$\boldsymbol{P}_i$ the Hill tensor depends on both the **shape and the conductivity of the matrix**.

For the case of an **oblate or prolate spheroidal inclusion in an isotropic matrix** of which the conductivity tensor has a simple form $\boldsymbol{\lambda}_0 = \lambda_0 \boldsymbol{\delta}$, the Hill tensor is expressed by (Giraud et al., 2007):

$$\boldsymbol{P} = \frac{Q}{\lambda_0}\left(\boldsymbol{\delta} - \underline{e}_3 \otimes \underline{e}_3\right) + \frac{1-2Q}{\lambda_0} \underline{e}_3 \otimes \underline{e}_3$$

$\underline{e}_3$ is the unit vector in the revolution direction of the ellipsoidal inclusion

Basis formulations of the homogenization method

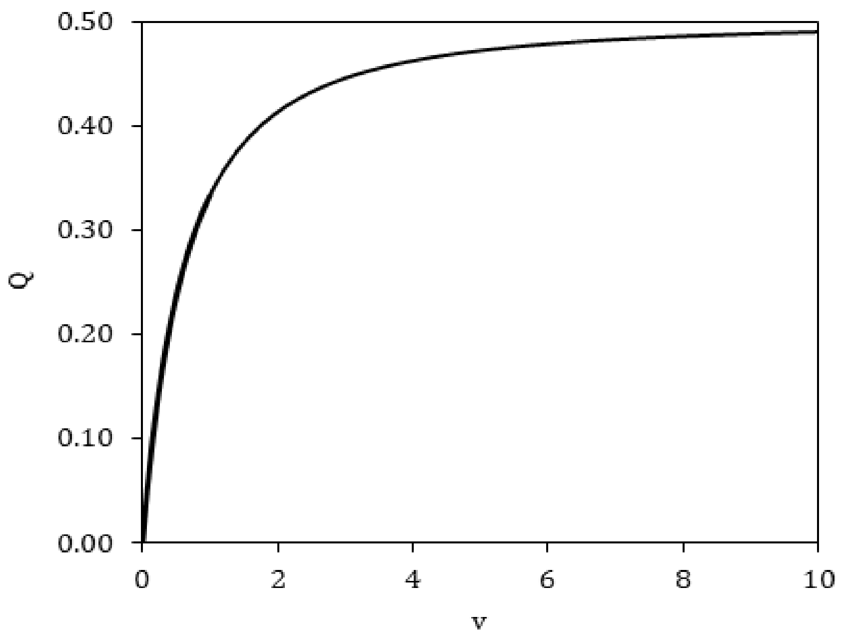
Parameter Q is a geometrical parameter that depends on:

$$\nu = X\sqrt{\lambda^T/\lambda^N} \qquad X^{hp} = \frac{l_{mean}}{\sqrt{w_{mean}e}}$$

with X, λ^T and λ^N are the aspect ratio and the conductivities of inclusion in transversal and normal directions

and for $\nu > 1$:

$$Q = \frac{1}{2} + \frac{2\sqrt{\nu^2-1} - \nu\ln\left(-1+2\nu^2+2\nu\sqrt{\nu^2-1}\right)}{4(\nu^2-1)^{3/2}}$$

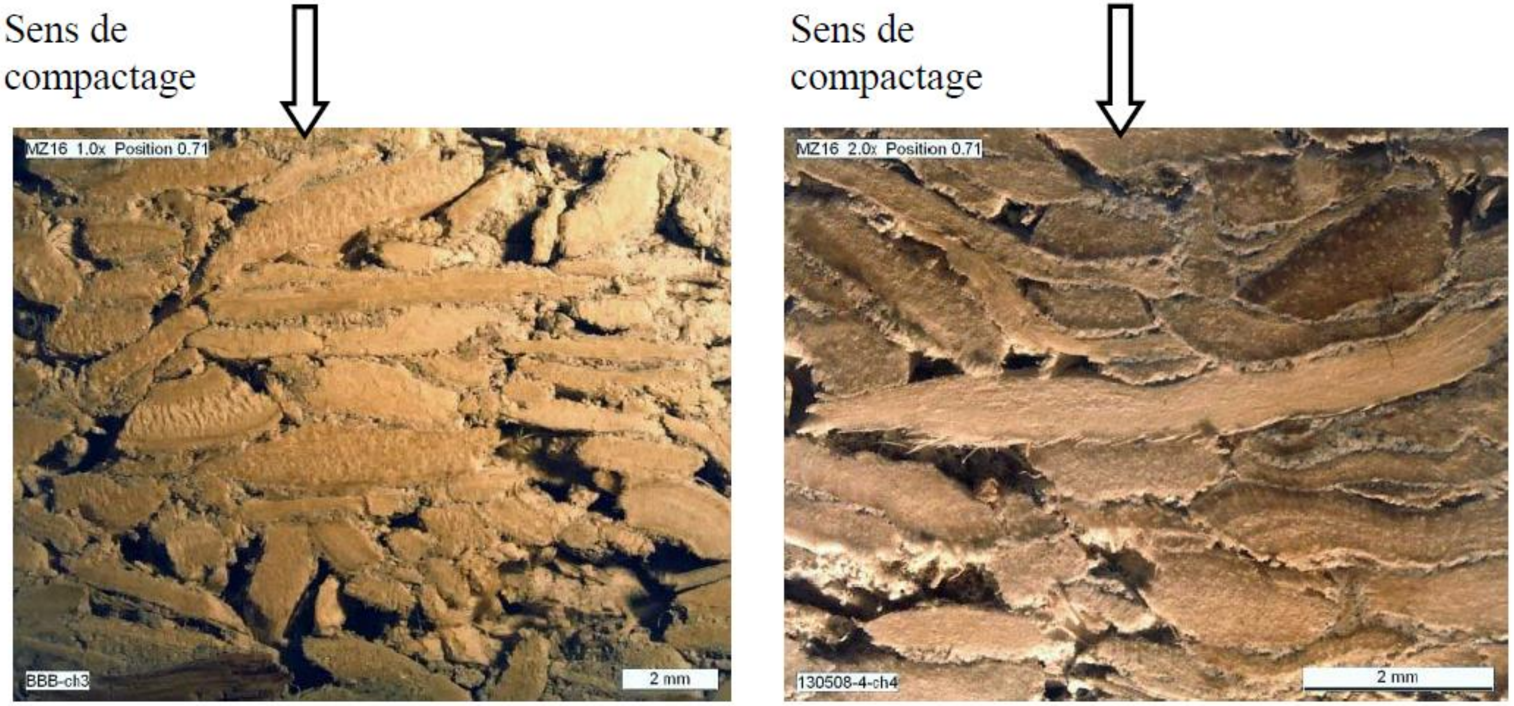


The parameter Q as function of the parameter ν

Example: for isotropic spherical inclusion: $\nu = X = 1$ and $Q = 1/3$.

Particle orientation distribution

Lime hemp concrete has an oriented internal structure that is determined by the direction of any compacting force and the degree of orientation of hemp particles depends on the production method.



(a) (b)

Observation des coupes verticales du béton de chanvre (Thèse NGUYEN Tai Thu, 2010)

Particle orientation distribution

Distribution function $W(\theta,\varphi)$ depends on the θ angle only and this function can take a form:

$$W(\theta,m) = (2m+1)\cos^{2m}\theta$$

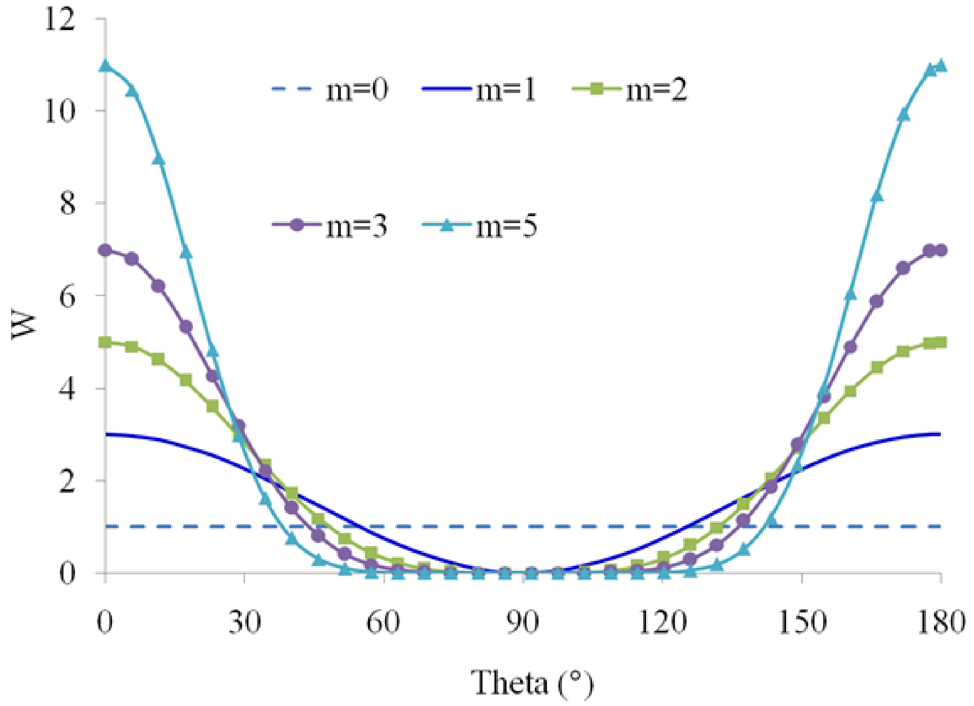
That satisfies the condition:

$$\frac{1}{2}\int_{\theta=0}^{\pi} W(\theta,m)\sin\theta\, d\theta = 1$$

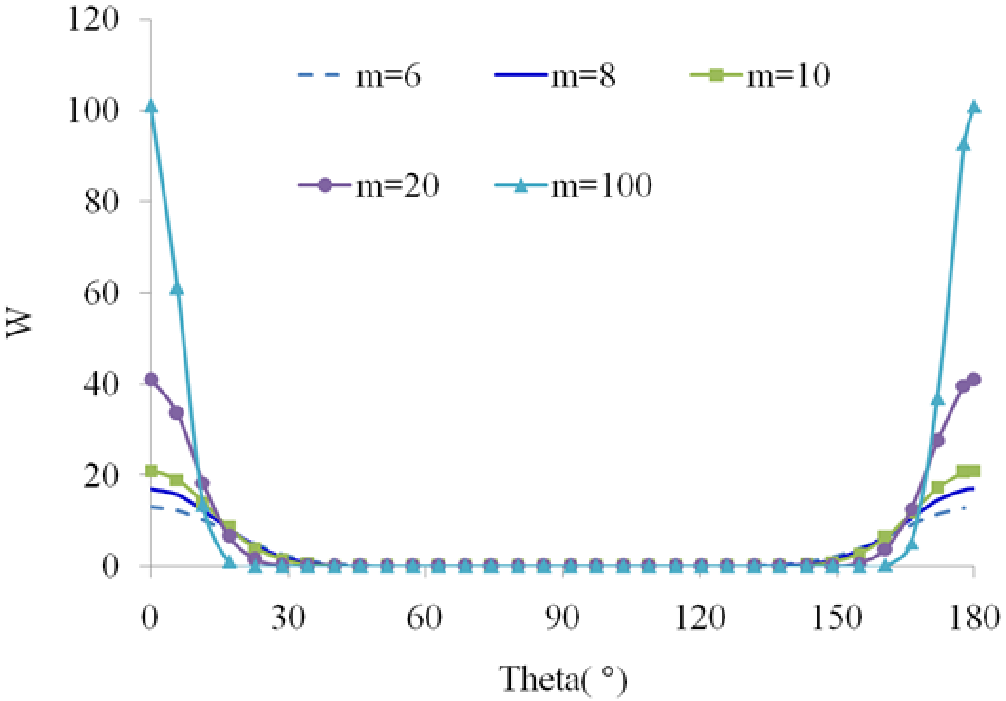
m is a distribution parameter that characterizes the degree of the preferred alignment distribution of the particles

θ is the angle between the axis of the pore and the global frame of the material.

Particle orientation distribution



Orientation distribution function
for m=0,1,2,3 and 5



Orientation distribution function
for m=6,8,10,20 and 100

Particle size distribution

Width

g(w) the probability density function and G(w) the probability that the width of a hemp shiv is equal or less than w

$$g(w) = a_w b_w w^{b_w - 1} \exp(-a_w w^{b_w})$$

$$G(w) = 1 - \exp(-a_w w^{b_w})$$

$$w_{mean} = \int_0^\infty w g(w) dw$$

To study the effect of the particle size of hemp particle, we define ***two probability density functions for the fiber length and fiber width distributions.***

$$f(l) = a_l b_l w^{b_l - 1} \exp(-a_l w^{b_l})$$

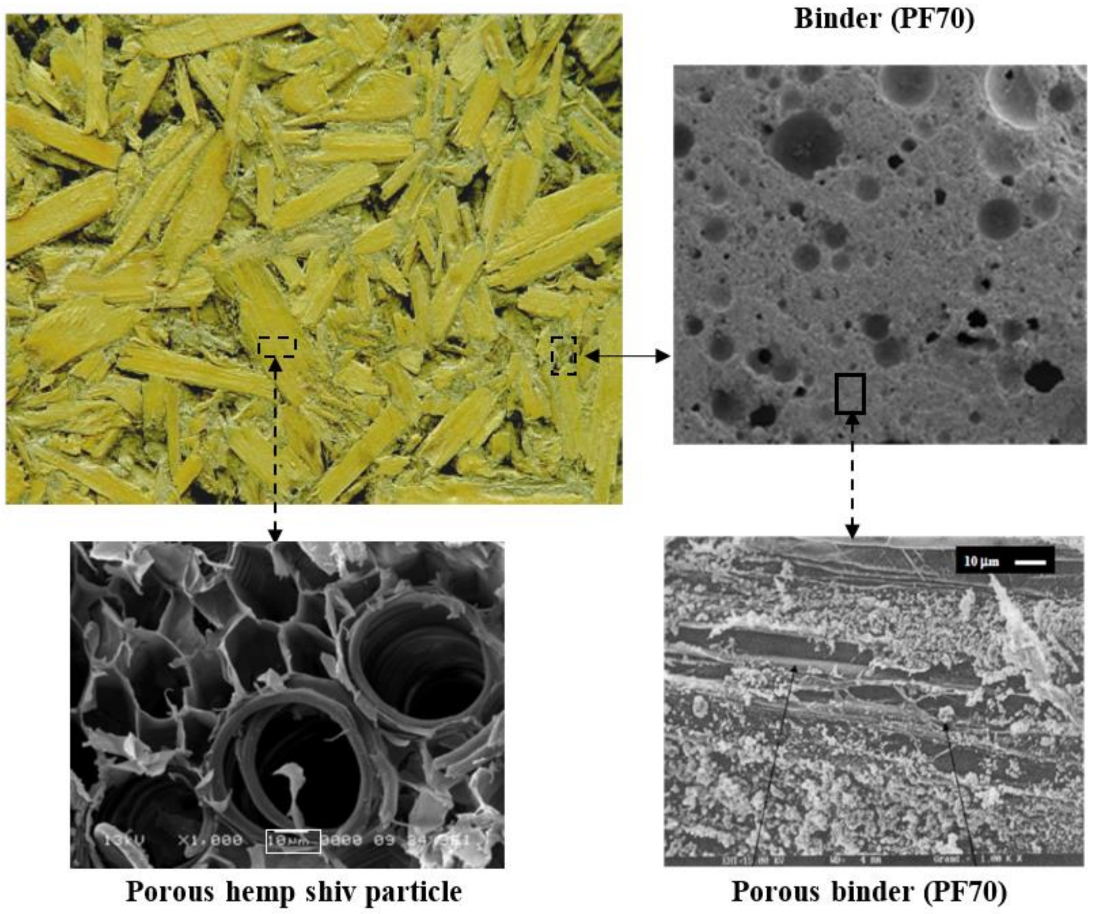
Length

$$l_{mean} = \int_0^\infty l f(l) dl$$

Two-scale homogenization approach

First scale: both the ***hemp particle and the binding phase*** are modeled as porous media.

Second scale (hemp concrete): a ***three phase mixture*** is considered: binding matrix, hemp particles (with and without imperfect interface) and macro pores



A two-scale homogenization approach based on microstructure and mesostructure of hemp concrete

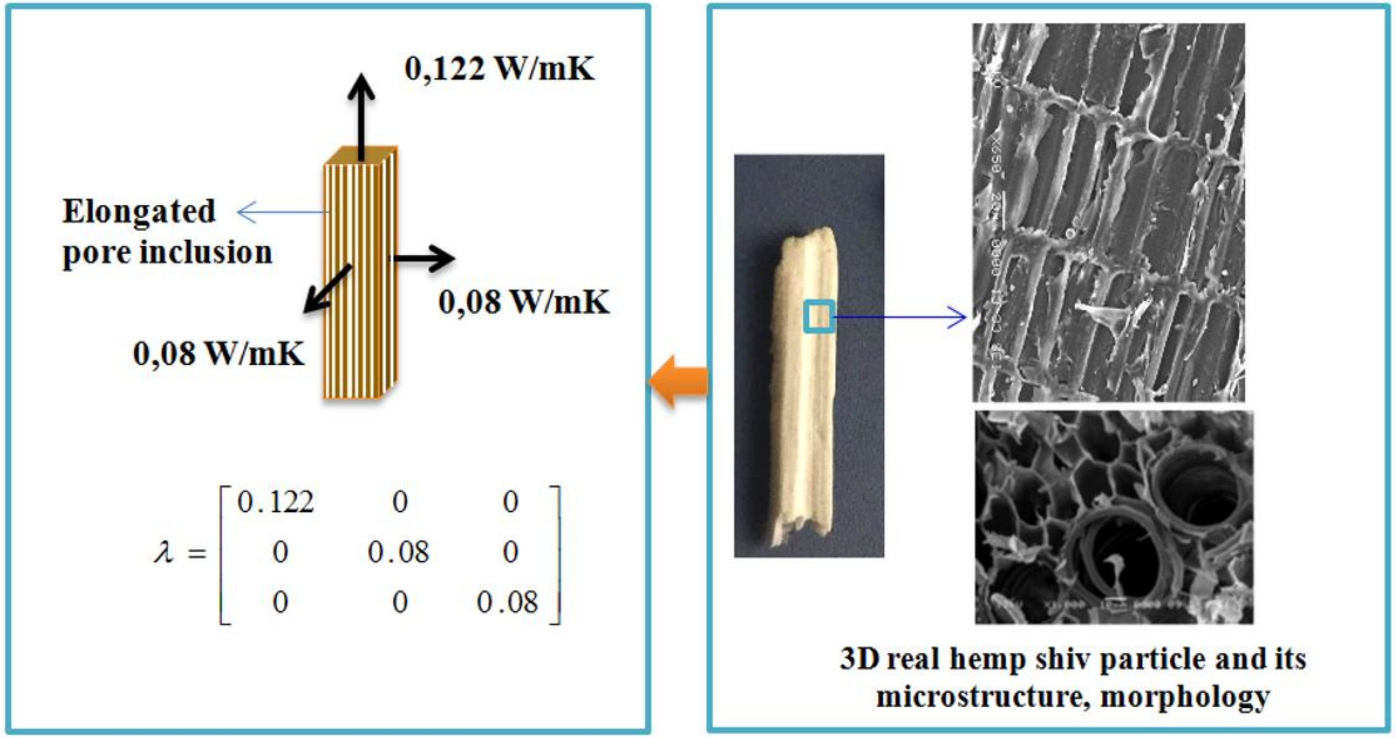
Effective thermal conductivity tensor of hemp shiv particle

$$\lambda_{hp}^{N} = \varphi_{hp}\lambda_a + (1 - \varphi_{hp})\lambda_s$$

$$\lambda_{hp}^{T} = \left(\frac{\varphi_{hp}}{\lambda_a + \lambda_s} + \frac{1 - \varphi_{hp}}{2\lambda_s}\right)^{-1} - \lambda_s$$

λ_a and λ_s the conductivity of air and the solid phases, respectively

φ_{hp} the porosity of hemp particle.



3D, microstructure and morphology of hemp shiv particle (right) and anisotropy of thermal conductivity tensor of a dry hemp shiv particle

Effective thermal conductivity tensor of dry binder

$$\lambda_b = \left(\frac{\varphi_b}{\lambda_a + 2\lambda_{bs}} + \frac{1-\varphi_b}{\lambda_{bs} + 2\lambda_{bs}} \right)^{-1} - 2\lambda_{bs}$$

λ_b and λ_{bs} are the overall conductivity and the conductivity of the solid phase of binder, respectively;

φ_b is the porosity of binder.

φ_b	λ_a (W/(m.K))	λ_b (W/(m.K))	λ_{bs} (W/(m.K))
0.506	0.0255	0.24	0.56

Conductivity of binder

Modeling imperfect thermal contact between hemp particles and surrounding binder

The imperfect interface contact between shiv and the binder has been highlighted and observed by scanning electron microscopy

The equivalent conductivity of a particle and its interface, noted by $\widetilde{\lambda}_{\mathrm{hp}}$: thermal jump across the interface to the macroscopic thermal gradient

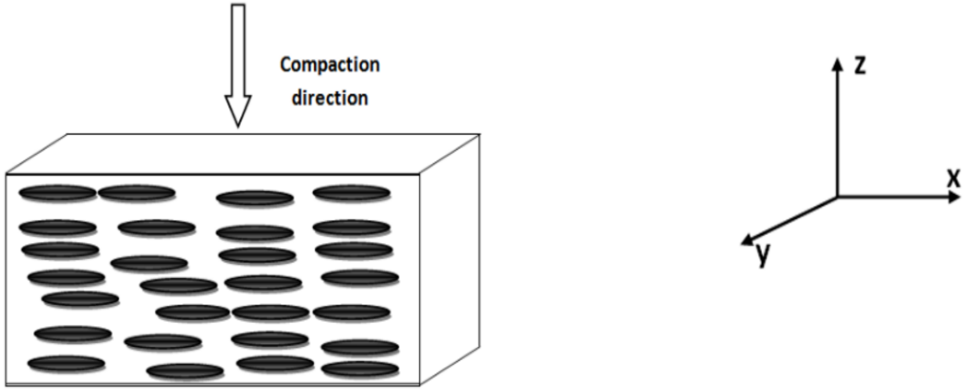
$$\tilde{\lambda}_{hp}^{T} = \frac{\lambda_{hp}^{T}}{1 + \alpha\, \lambda_{hp}^{T}/\lambda_{b}}\,;\ \tilde{\lambda}_{hp}^{N} = \lambda_{hp}^{N}$$

λ_b the thermal conductivity of the surrounding binding matrix that is assumed to be isotropic;

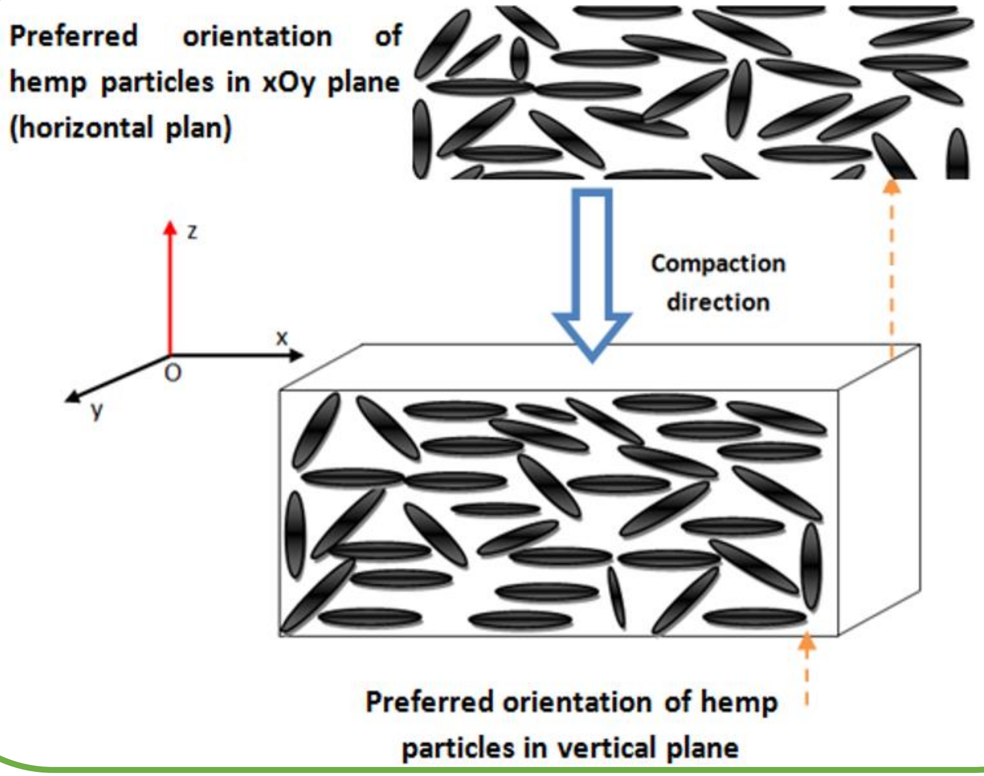
α interface parameter that characterizes the thickness, the thermal conductivity of the interface zone.

α is considered as an intrinsic parameter that will be calibrated by an inverse analysis using experimental data.

Effective thermal conductivity tensor of dry hemp concrete



Perfect alignment of hemp particles in the horizontal plan

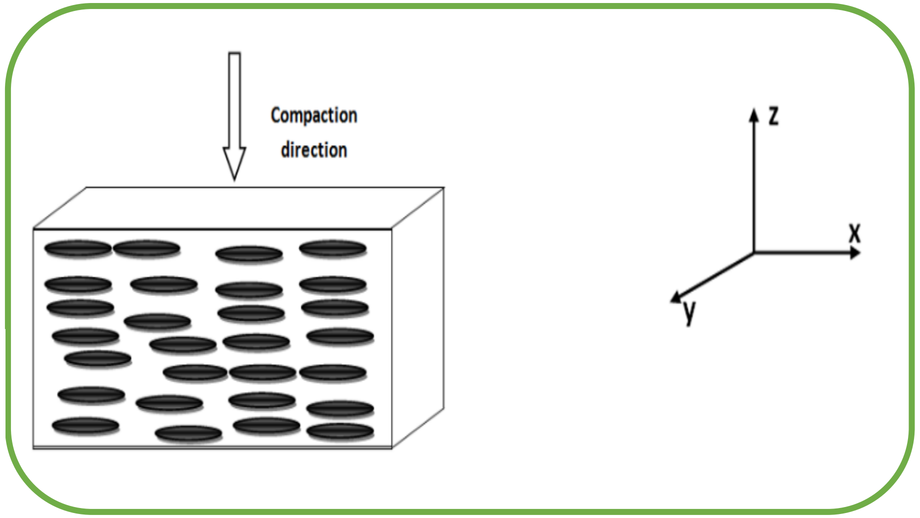


Preferred spatial orientations in different planes (horizontal and vertical planes) for developing model

Effective thermal conductivity tensor of dry hemp concrete: *Perfect alignment model*

$$\lambda_{hom}^{T} = \frac{(1-f_a-f_{hp})\lambda_b + f_a\lambda_a \frac{3\lambda_b}{\lambda_a+2\lambda_b} + f_{hp}\frac{\tilde{\lambda}_{hp}^{T}\lambda_b}{Q(\tilde{\lambda}_{hp}^{T}-\lambda_b)+\lambda_b}}{(1-f_a-f_{hp}) + f_a \frac{3\lambda_b}{\lambda_a+2\lambda_b} + f_{hp}\frac{\lambda_b}{Q(\tilde{\lambda}_{hp}^{T}-\lambda_b)+\lambda_b}}$$

$$\lambda_{hom}^{N} = \frac{(1-f_a-f_{hp})\lambda_b + f_a\lambda_a \frac{3\lambda_b}{\lambda_a+2\lambda_b} + f_{hp}\frac{\tilde{\lambda}_{hp}^{N}\lambda_b}{(1-2Q)(\tilde{\lambda}_{hp}^{N}-\lambda_b)+\lambda_b}}{(1-f_a-f_{hp}) + f_a \frac{3\lambda_b}{\lambda_a+2\lambda_b} + f_{hp}\frac{\lambda_b}{(1-2Q)(\tilde{\lambda}_{hp}^{N}-\lambda_b)+\lambda_b}}$$



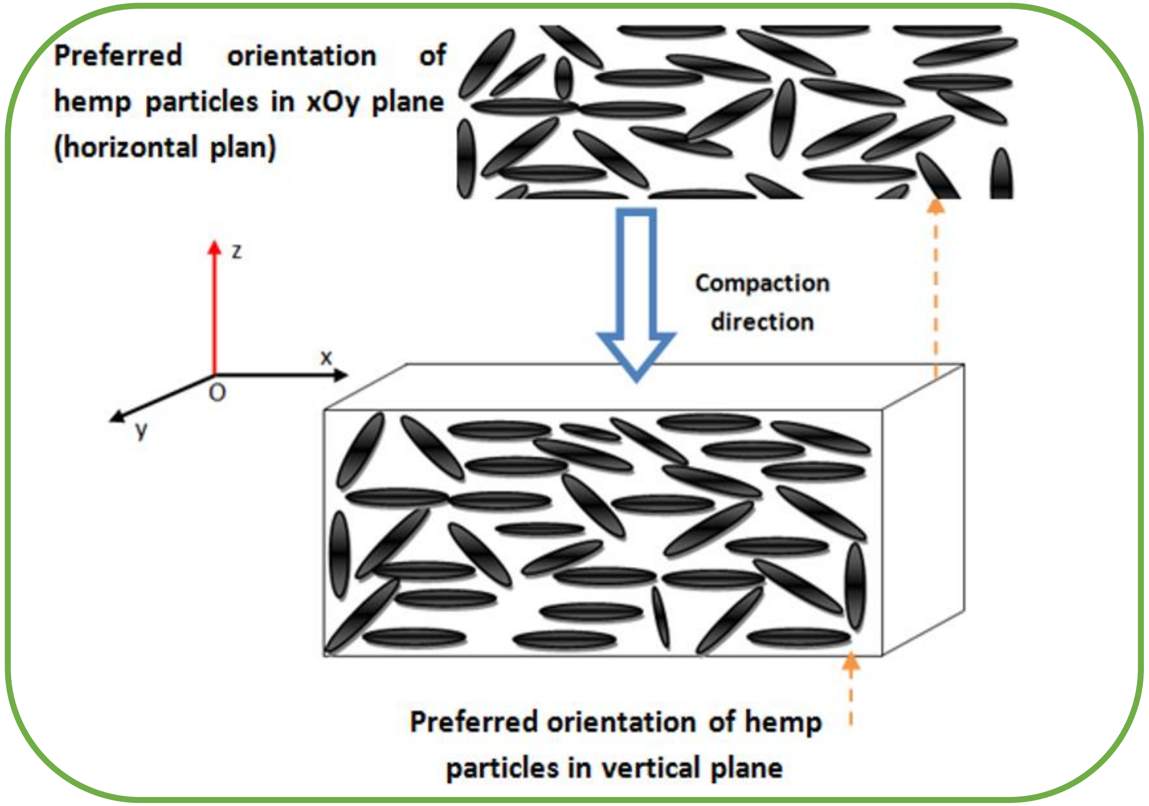
Perfect alignment of hemp particles in the horizontal plan

$$\boldsymbol{\lambda}_x = \begin{bmatrix} \lambda_{xx} & 0 & 0 \\ 0 & \lambda_{yy} & 0 \\ 0 & 0 & \lambda_{zz} \end{bmatrix} = \begin{bmatrix} \lambda_{al}^{N} & 0 & 0 \\ 0 & \lambda_{al}^{T} & 0 \\ 0 & 0 & \lambda_{al}^{T} \end{bmatrix}$$

Effective thermal conductivity tensor of dry hemp concrete: *preferred spatial orientations model*

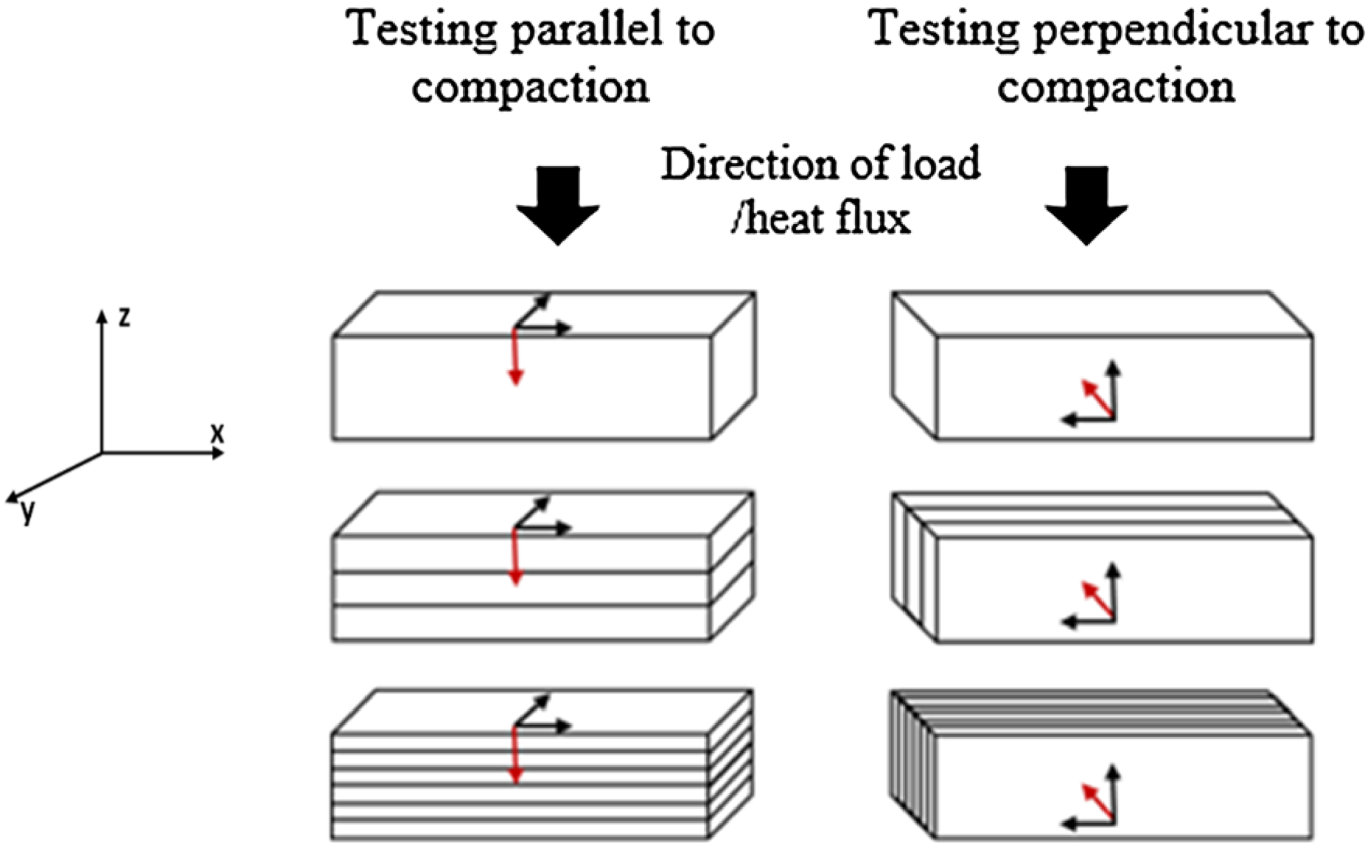
$$\langle \boldsymbol{\lambda}^{\varphi\theta}{}_{hom} \rangle = \begin{bmatrix} \frac{2m+1}{2(2m+3)}\lambda_{al}^{N} + \frac{2m+5}{2(2m+3)}\lambda_{al}^{T} \\ \frac{1}{2}(\lambda_{al}^{N} + \lambda_{al}^{T}) \\ \frac{1}{2m+3}\lambda_{al}^{N} + \frac{2m+2}{2m+3}\lambda_{al}^{T} \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \lambda^{\varphi\theta}_{xx\ hom} \\ \lambda^{\varphi\theta}_{yy\ hom} \\ \lambda^{\varphi\theta}_{zz\ hom} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- Random orientation distribution: $m = 0$ isotropic average tensor $\langle \boldsymbol{\lambda} \rangle$.
- Aligned distribution, $m \to \infty$, $\langle \boldsymbol{\lambda} \rangle = \boldsymbol{\lambda}$.



Preferred spatial orientations in different planes (horizontal and vertical planes) for developing model

Model validation



Testing direction arrangements for parallel and perpendicular loading with direction of compaction and preferred plane of orientation of particles indicated by the red and black axis respectively

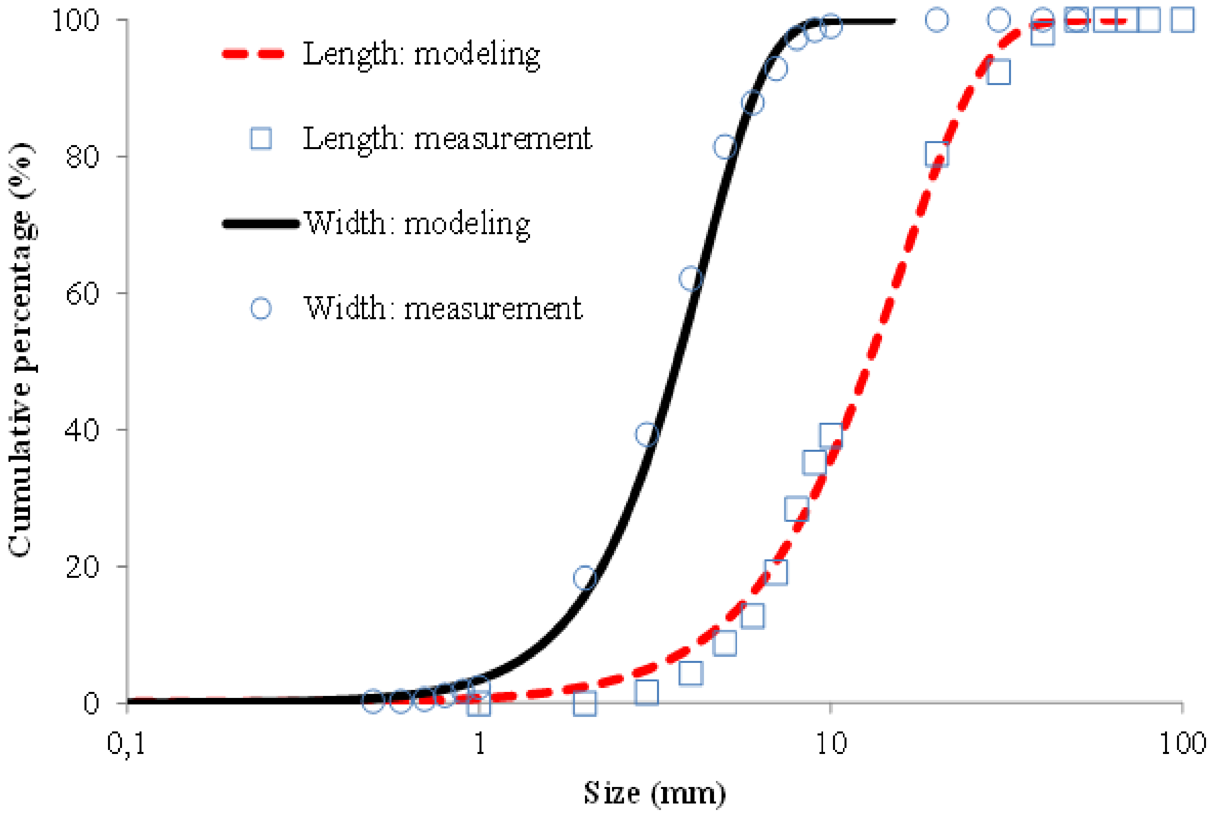
(source: Williams et al., 2017).

Model validation

Size distribution of hemp shiv particles

a_w	b_w	w_{mean} (cm)
0.035	2.3	0.38

a_l	b_l	l_{mean} (cm)
0.07	1.8	1.4



Computed and measured values of cumulative distributions of lengths and widths of hemp shiv particles

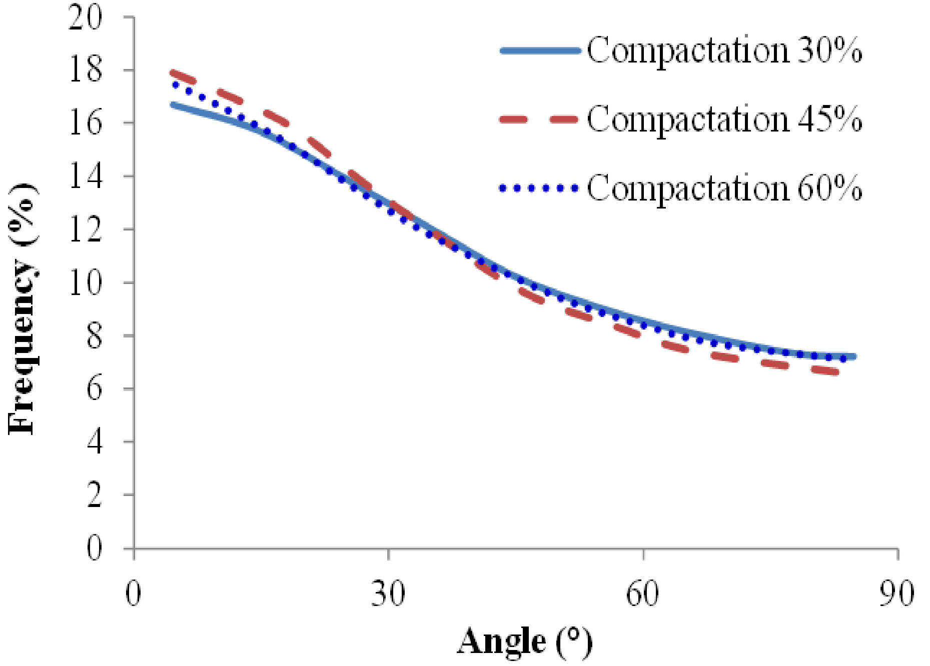
Model validation

Oriented distribution of hemp particles

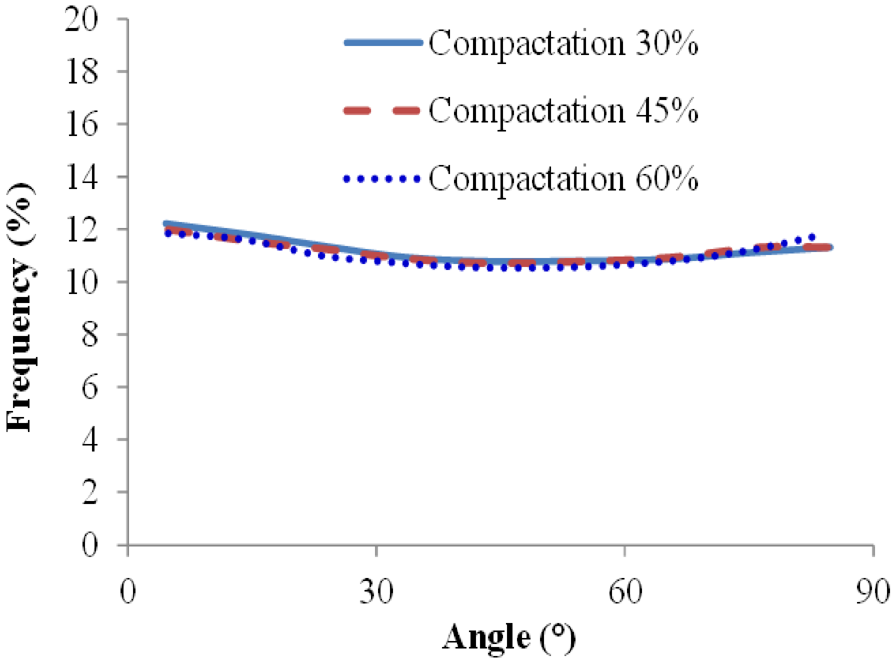
Internal structure : A novel application of image analysis methodology developed by *Williams et al. (2017)*

- Frequency distributions of particle orientation
- Three compaction levels: 30, 45 and 60% volumetric decrease from the uncompact state

Distribution parameter (m value)=1



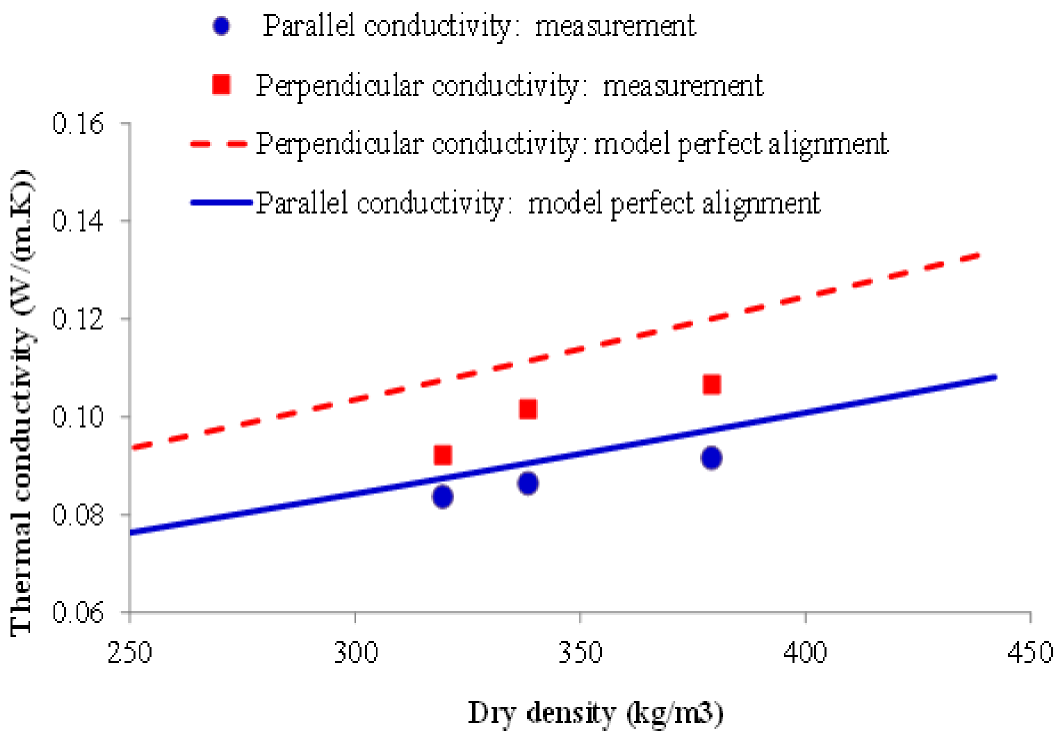
Perspective perpendicular to compaction



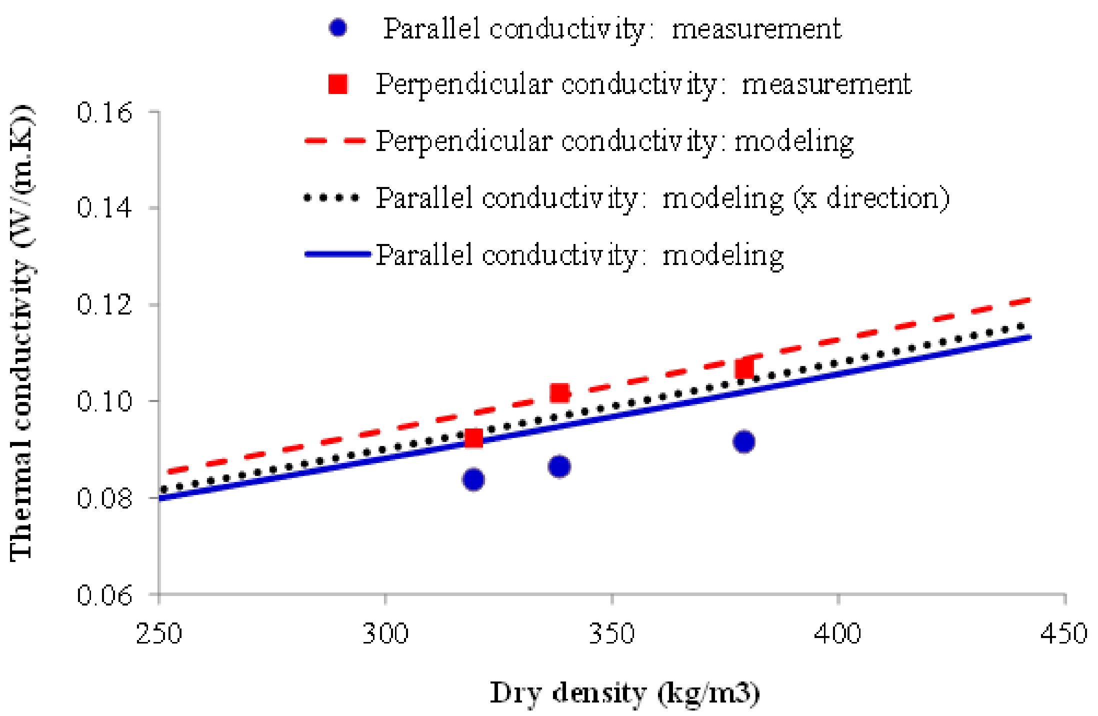
Parallel to compaction

Model validation

Perfect alignment vs Preferred spatial orientations models



Perfect alignment model



Preferred spatial orientations model

Model validation

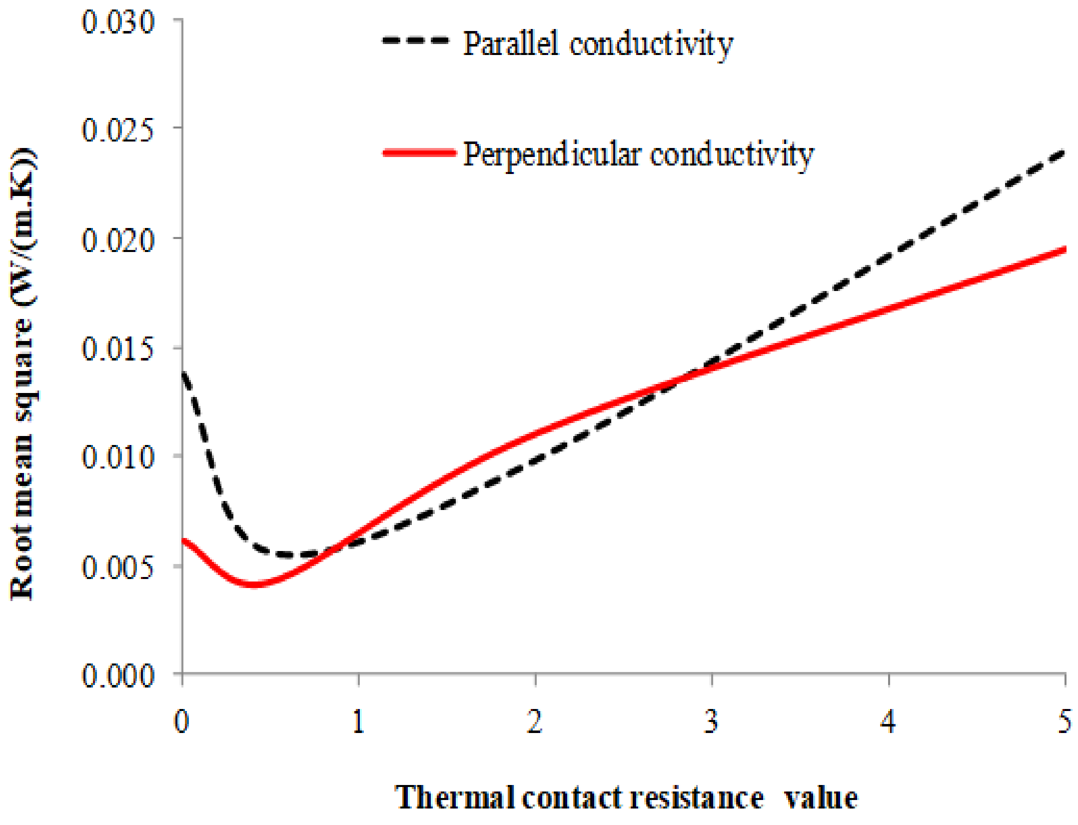
Impact of imperfect thermal interface

Root mean square difference (*gamma*)

$$\Gamma_{RMS} = \sqrt{\frac{\sum_{n=1}^{N} (\Delta\lambda)^2}{N}}$$

Δλ: difference thermal conductivity between the measured and predicted values,

N: number of values in the data set

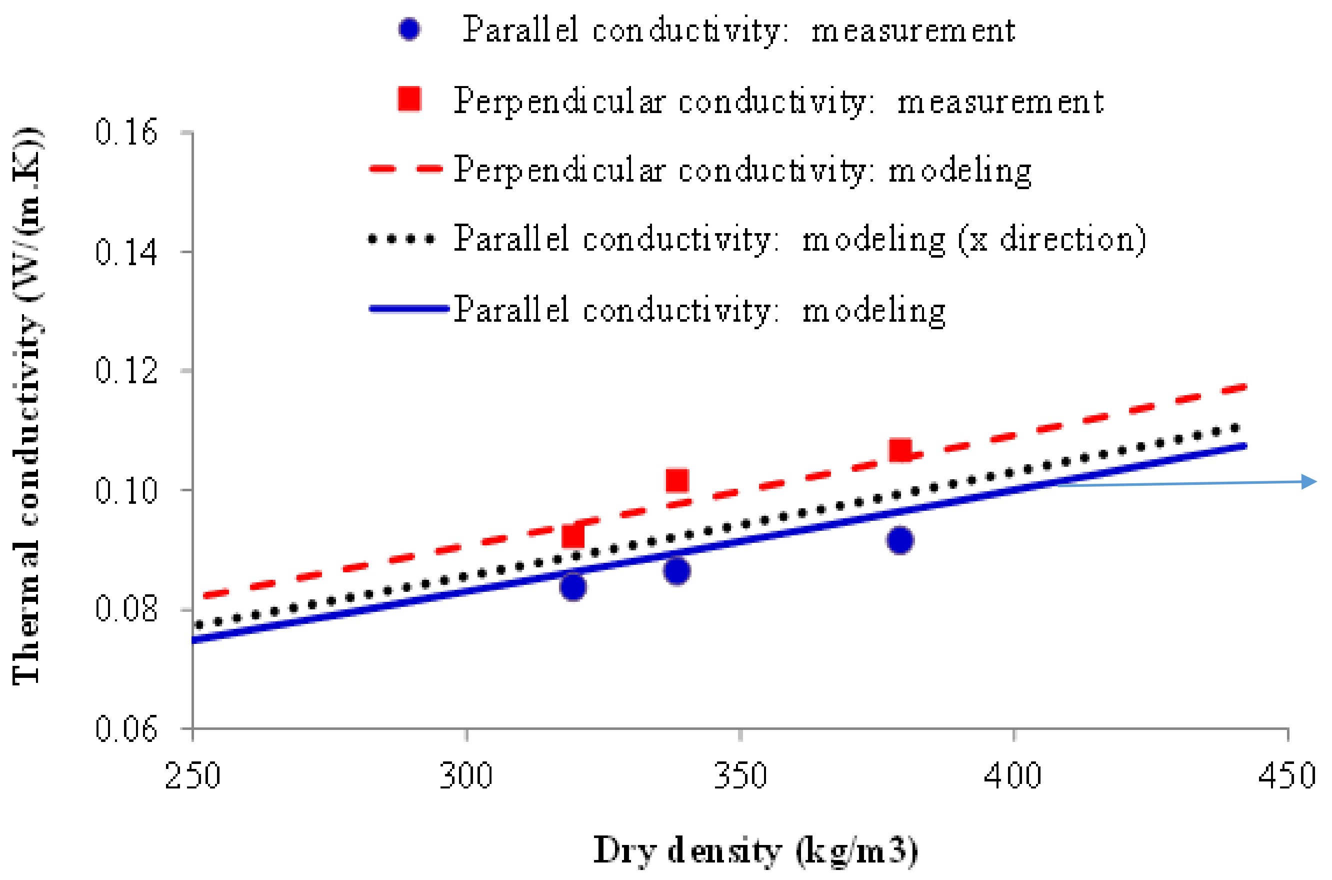


Effect of thermal interface contact resistance (α) on the root mean square difference

α=0.5 : smallest values of Γ_{RMS} values of both conductivity components

Model validation

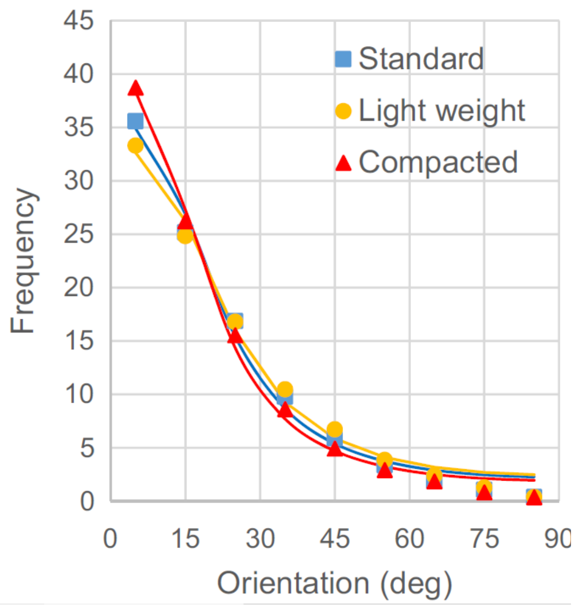
Preferred spatial orientations model with imperfect thermal interface (α=0.5)



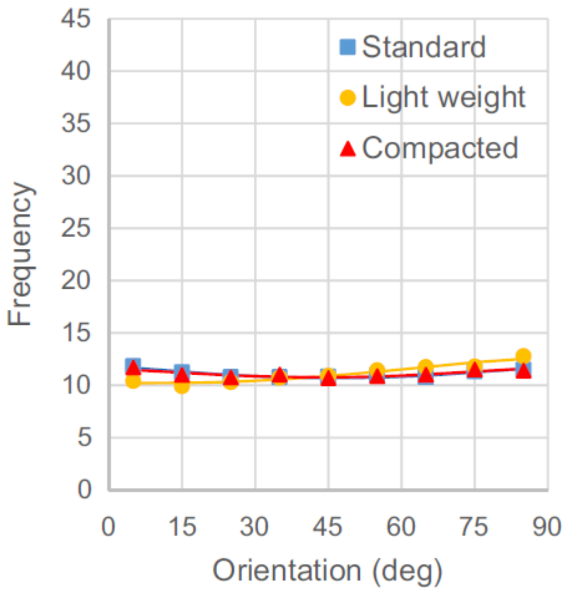
the modelling consistently over-predicts for parallel direction

Model validation

Two method to determine the oriented distribution of hemp particles*



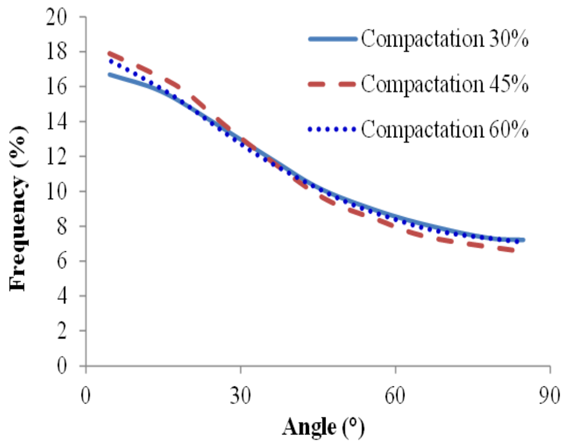
Perpendicular to compaction



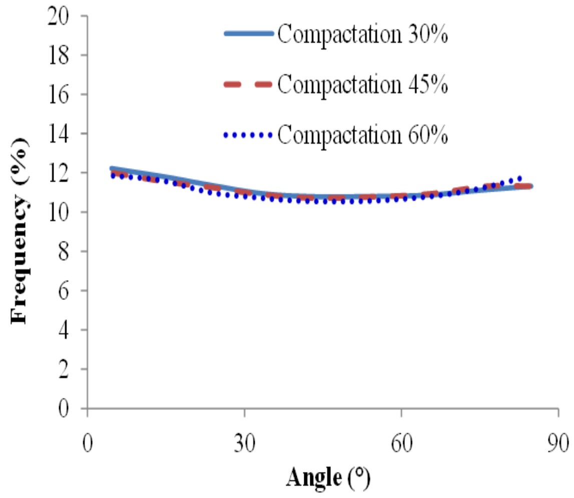
Parallel to compaction

Computer tomography scanning (CT scanning)

Distribution parameter (m value)=3



Perpendicular to compaction



Parallel to compaction

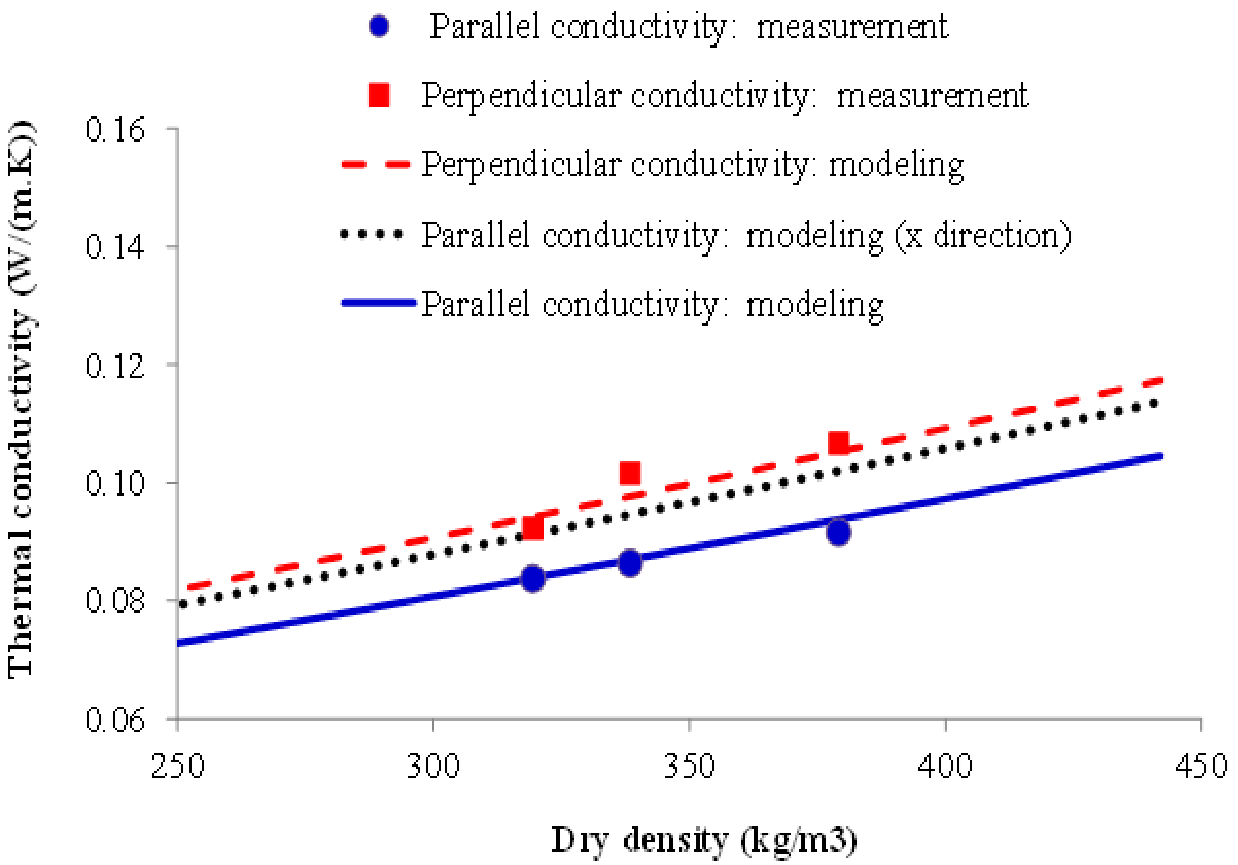
Visual digital imaging method

Distribution parameter (m value)=1

*Source: *Williams, J., Lawrence, M., Walker, P. A method for the assessment of the internal structure of bio-aggregate concretes. Construction and Building Materials, 116, 2016, 45–51.*

Model validation

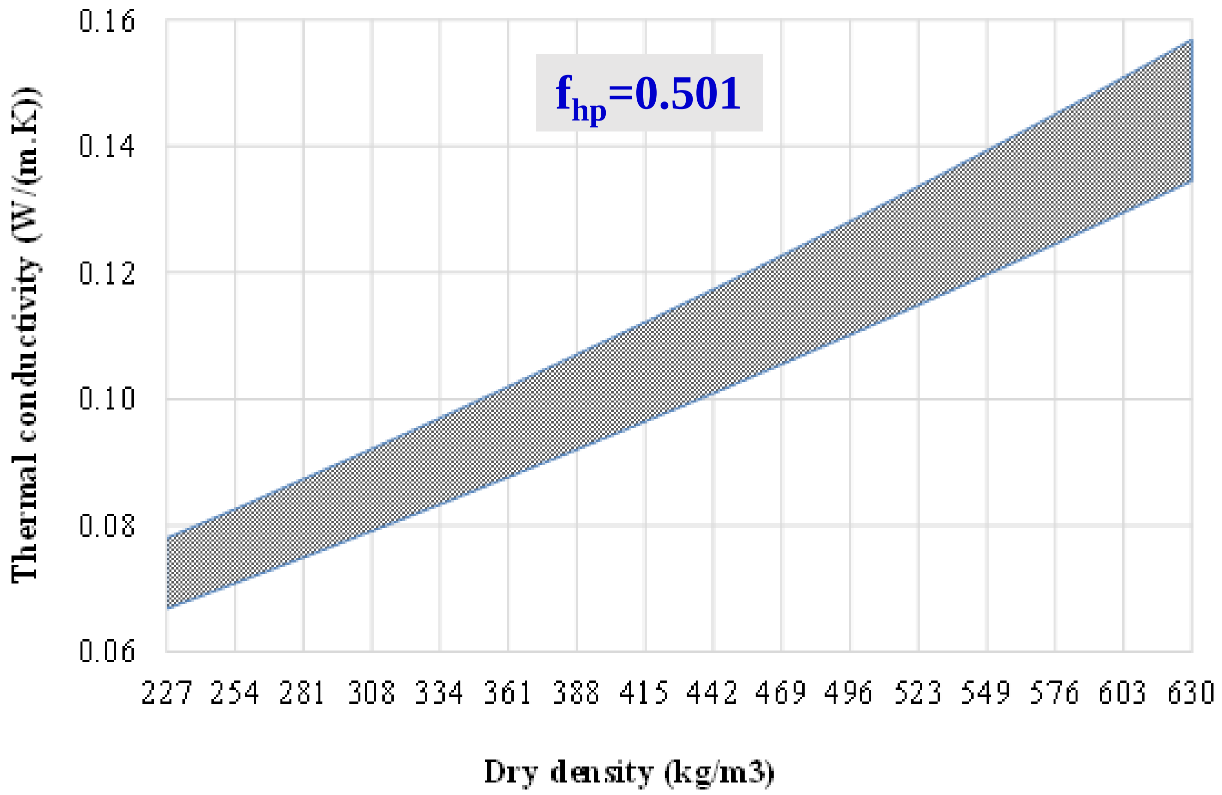
Distribution parameter (m value)=3



Computed values and measured thermal conductivities with m=3 based on the results obtained from CT scanning method (Williams et al., 2016).

Application example

The range of thermal conductivity of hemp concrete in different direction



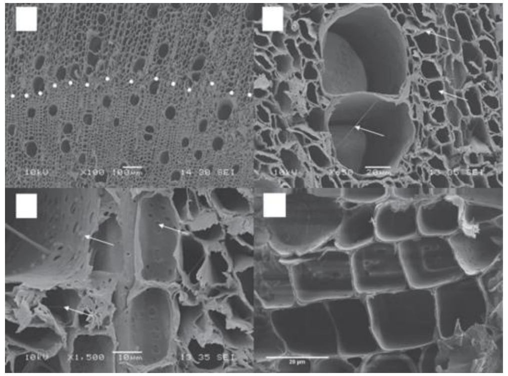
The range of the thermal conductivity of hemp concrete depending on the measured direction when m value varies between 0 and ∞.

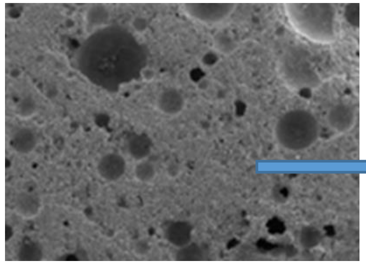
Use of the developed model

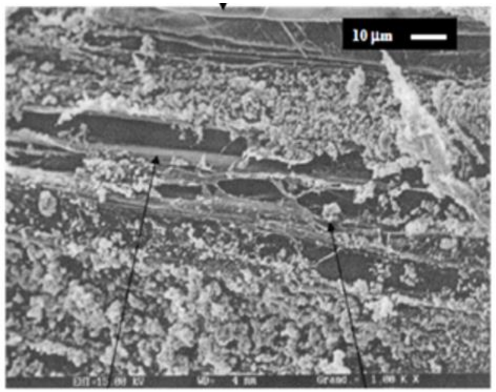
Many parameters have been taken into account in only one model to optimize the effective thermal conductivity of hemp concrete

- **Hemp shiv particles**: defined by *λs* (conductivity of solid phases of hemp shiv), *φhp* (porosity of hemp particle) and the hemp shiv size distribution function.
- **Hemp shape and the anisotropy:** of the inclusion: the Q, a and b parameters introduced in the model.
- **Binder type**: it is defined by λbs (solid phase of binder) and ϕb (porosity of binder).

Components of hemp concrete







Porous binder (PF70)

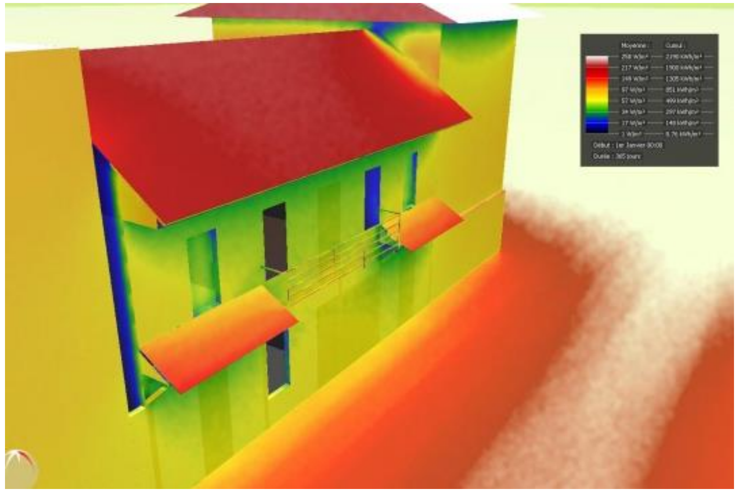
Use of the developed model

Many parameters have been taken into account in only one model to optimize the effective thermal conductivity of hemp concrete

- **Formulation of hemp concrete**: f_{hp} (volume fraction of hemp particles) and f_b (volume fraction of binder).
- **Manufacturing process**: the distribution parameter m determined based ***on the image analysis technique*** (CT imaging and VD imaging methods as presented in *Williams et al., 2016; 2017*).
- **Durability and surface treatment**: an interface parameter α, imperfect thermal contact between hemp particles and surrounding binder (can appear during drying period, surface treatment or the aging).

Use of the developed model

- Very good analytical tool to investigate the variability of the thermal conductivity of hemp concrete.
- Effect of one parameter on the overall thermal conductivity of hemp concrete can be quickly assessed and predicted (when it is not possible to quantify experimentally due to the technical problems such as measurement precision errors of the testing apparatus).
- Presented analytical solutions offer potential opportunities for using 3D thermal simulation tools to optimize hemp-building performance.



Conclusion

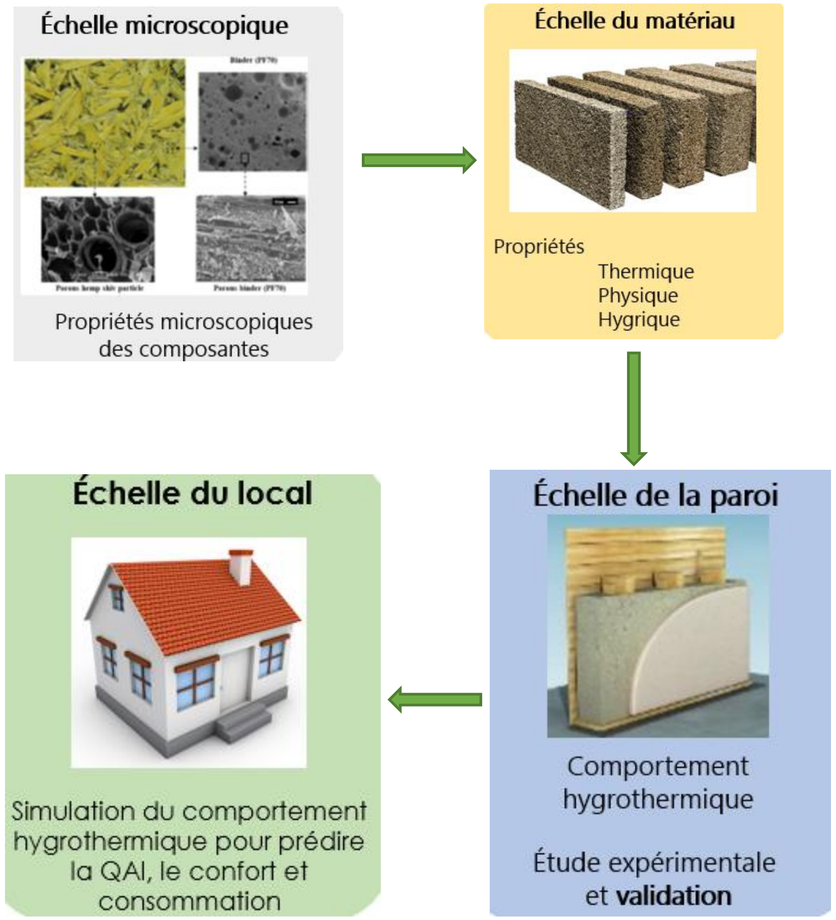
Anisotropy of the thermal conductivity of hemp concrete: the thermal conductivity components are different in different direction

Anisotropy can be strongly modified by the ***manufacturing process***.

The CT scanning method is a suitable method for the assessment of hemp concrete.

The novel mathematical model developed is very useful to **optimize the thermal performance of bio-based materials** such as hemp concrete and building design.

For future works, the developed model will be extended and developed for **multi-scale study** focusing on **hygrothermal behavior of hemp concrete** from **micro scale to higher scale levels**: such as materials, building envelope and buildings.



For future works