Thermal conductivity calculation of bio-aggregates based materials using finite and discrete element methods

Fabienne Pennec, Arnaud Alzina, Nicolas Tessier-Doyen, Benoit Naitali, David S Smith
GEMH-CEC, 12, rue Atlantis, 87068 Limoges Cedex, France
E-mail: fabienne.pennec@unilim.fr

Abstract. This work is about the calculation of thermal conductivity of insulating building materials made from plant particles. To determine the type of raw materials, the particle sizes or the volume fractions of plant and binder, a tool dedicated to calculate the thermal conductivity of heterogeneous materials has been developed, using the discrete element method to generate the volume element and the finite element method to calculate the homogenized properties. A 3D optical scanner has been used to capture plant particle shapes and convert them into a cluster of discrete elements. These aggregates are initially randomly distributed but without any overlap, and then fall down in a container due to the gravity force and collide with neighbour particles according to a velocity Verlet algorithm. Once the RVE is built, the geometry is exported in the open-source Salome-Meca platform to be meshed. The calculation of the effective thermal conductivity of the heterogeneous volume is then performed using a homogenization technique, based on an energy method. To validate the numerical tool, thermal conductivity measurements have been performed on sunflower pith aggregates and on packed beds of the same particles. The experimental values have been compared satisfactorily with a batch of numerical simulations.

1. Introduction
The use of building materials, that complies with legislations and users actual requirements concerning environmental and health impacts as well as thermal or hygroscopic comfort, is recently growing by leaps and bounds. In this context, original thermal insulating panel for the existing building and with low environmental impact are developed. These building materials are made from vegetable particles, obtained from grinding of plants non recycled by agriculture, renewable and easily available, as maize or sunflower. The particles will be used as aggregates in combination with one biodegradable binder, from plant or animal origins.
To meet the expectations of optimizing the insulating material for its thermal, mechanical and hygroscopic performances, organic raw material characterization is first performed. The composite material composed of both vegetable particles and one organic binder is also subsequently tested. This last objective is complex to achieve accurately because of the existence of many influencing parameters, such as the nature of the organic raw material and of the organic binder, the particle shape, size and orientation, the particle and binder volume fraction or the pressure applied to pack down the mixture. To evaluate the impact of these different parameters without carrying out substantially expensive experimental investigations, the material behavior is sim-
ulated using 3D finite element analysis on a statistically representative geometry entity of the organic mixture, referred to as Representative Volume Element (RVE).

The plant material considered in this paper is pith extracted from sunflower stems. The particles are in the form of particular grains, with sizes varying from 0.5 to 10mm (Figure 1). The final product exhibits a large volume fraction (60-90%) of these plant particles to ensure a sufficiently high mechanical resistance. The main difficulty in analysing the building material behavior lies in the modeling of the geometry at the micro-level for high particle volume ratios. The microscale geometry generation algorithm which is widely used for studies of particle packing or particle reinforced composites is a random sequential adsorption algorithm (RSA) [14, 6]. This algorithm consists indeed in adding aggregates sequentially into a volume element by randomly generating the center point and two Euler angles. Intersections of any two aggregates is forbidden. Therefore, even if the RSA algorithm can consider various particle shapes, the maximum achievable aggregate volume fraction is limited to about 35-40%.

Instead of using traditional adsorption algorithms, a Discrete Element Method (DEM) is employed to dynamically build the RVE, virtually recreating the manufacturing process.

2. Generation of 3D RVE using DEM

In practice, it would be computationally impossible to generate geometries depicting the entire sample containing multiple plant particles with various shapes. In this case, the notion of RVE is used. The RVE is regarded as the minimal volume of the heterogeneous material used for the evaluation of the effective thermal conductivity. As a result the volume must be sufficiently large to be statistically representative of the multi-phase material but also permit the morphology of microstructural heterogeneities to be described in sufficient detail.

2.1. RVE generation protocol

The Discrete Element Method (DEM) is a numerical technique, in which Newton’s second law and a finite difference scheme are used to study the interaction among discrete particles in contact. The contact between any two particles can be represented through springs and dashspots. The dynamic process is completed through the integration of particles’ acceleration and velocities with an explicit time stepping algorithm. In this technique, Newton’s law of motion is successively solved for each particle and force-displacement law is applied for every contact. Newton’s second law is used to calculate the particle’s acceleration, resulting from the contact and external forces. The force-displacement law is used to update the contact forces resulting from the overlap of the two contacting particles. These two laws are applied successively to form the whole computation cycle of DEM. DEM is thus particularly suitable to simulate the dynamic behaviour of a granular system, in which the motion of every particle is recorded and analysed over each time step [2, 12]. Today, the discrete particles can also be densely packed and bonded together by adding special bonds at the contact points [7]. This method is used to simulate solid materials of various shapes.

Therefore, in the present study, the DEM is carried out to simulate the filling of a container by a cluster of plant aggregates, modeled themselves by clusters of discrete elements. These aggregates are initially randomly distributed but without any overlap, and then fall down in a container due to the gravity force and collide with neighbour particles according to a velocity Verlet algorithm [15]. In addition an oscillating displacement is imposed to the container to optimize the natural spatial arrangement of the aggregates in the container. An open-source free software (GranOO workbench) dedicated to 3D dynamic simulations based on the DEM, has been used to support the development of the algorithm by adding processed plugins within software.
2.2. Plant particles generation

Most of the 3D DEMs use spherical elements, because only the radius is required to define the particles geometry and there is only one possible type of contact among particles, which can be detected easily. As a result, computer memory requirements and computer processing time are minimized and a large number of particles can be studied. However, the actual analyzed particles exhibit various shapes and considering them as spherical elements doesn’t allow to reach the large particle volume fraction expected in the building materials. Even if more complex shapes, such as polyhedrons, can be built, detecting contacts and calculating forces and torque are more difficult in this case[13]. Another solution is to model these shapes by clumps of spheres bonded together. Even if this method requires a larger number of elements, the contacts are more readily solved in clusters as compared to polyhedrons, and the calculation cost remains reasonable.

A reverse engineering method is used to build the 3D CAD model of a real vegetable particle (Figure 1). 3D scanners are used to capture the particle shape and generate a high resolution model. 3D Optical scanning systems can capture millions of points in a second to create point clouds data. The resulting 3D data is then transferred to a surface reconstruction software to eliminate outlier and reduce noise. The modeling software exports models in ascii format, which are used as input to the CGAL open-source project. The Computational Geometry Algorithms Library (CGAL) offers data structures and algorithms like surface reconstruction from point sets (Figure 2) and 3D mesh generation of polyhedral surfaces, which allows the 3D meshing of the 3D CAD model (Figure 3). The generated meshing is then used to build the discrete domain with discrete elements set at the mesh nodes (Figure 4) and with added bonds corresponding to the different meshes. The regular meshing generated by CGAL algorithm permits to obtain discret objects homogeneously filled with the discrete elements.

Figure 1. Picture of sunflower pith aggregate.

Figure 2. CGAL surface reconstruction from point sets.

Figure 3. CGAL 3D mesh generation.

Figure 4. Aggregate modeled with a mesh of small DEs.

2.3. RVE generation in the SALOME platform

Once the DEM computation performed and the vegetable particles fallen down in the container, the geometry is converted in a python script to be generated in the open-source Salome software (Figures 5 and 6). A cubic RVE is then clipped in the assembly and the aggregate volume fraction calculated (Figures 7, 8 and 9).
The cubic volume element is very complex from a geometrical point of view. This causes difficulties in the meshing of the cubic element. In this way, only cubic volume elements of about 5mm size have been built and meshed. To determine the effective properties of such small volumes, a sufficient number of realizations has to be considered according to Kanit et al. [8]. For a given aggregate volume fraction, a dozen of representative volume elements has been therefore generated and used to calculate the effective thermal conductivity via the homogenization technique.

![Figure 5](image1.png)  
**Figure 5.** DEM computation in process with 460 vegetable particles.

![Figure 6](image2.png)  
**Figure 6.** DEM computation final step with 460 vegetable particles.

![Figure 7](image3.png) 
**Figure 7.** RVE with 63% of aggregate volume fraction.

![Figure 8](image4.png) 
**Figure 8.** RVE with 82% of aggregate volume fraction.

![Figure 9](image5.png)  
**Figure 9.** RVE with 89% of aggregate volume fraction.

3. Implementation of thermal homogenization technique

3.1. Principle of the homogenization method

A homogenization technique with a uniform temperature gradient at the boundary [1] has been implemented in the finite element code to execute the calculations of the effective thermal conductivity.

The main objective of the homogenization method is to find a homogeneous volume equivalent to the original heterogeneous volume, where the thermal energy stored in both systems is approximately the same. The averaged microscopic energy is calculated by integration over the unit cell volume \( V \):

\[
2W_I = \frac{1}{V} \int q \cdot \nabla T dV = \langle q \cdot \nabla T \rangle_V
\]  
(1)
$\mathbf{q}$ is the heat flux density vector and $\nabla \mathbf{T}$ is the temperature gradient vector. It is useful to decompose $\mathbf{q}$ and $\nabla \mathbf{T}$ into their average and fluctuating components, where the average of the fluctuating part is zero. Hill’s theorem [5] relates the macroscopic values to microscopic ones:

$$\langle \mathbf{q} \cdot \nabla \mathbf{T} \rangle_V = \langle \mathbf{q} \rangle_V \cdot \langle \nabla \mathbf{T} \rangle_V$$  (2)

and

$$\langle \mathbf{q} \rangle_V = \langle \nabla \mathbf{T} \cdot \mathbf{A} \rangle_V = \langle \nabla \mathbf{T} \rangle_V \cdot \langle \mathbf{A} \rangle_V$$  (3)

Accordingly the macroscopic energy is equal to the average of the microscopic energy. The macroscopic energy is defined by treating the heterogeneous material as a homogeneous material with uniform field $\langle \nabla \mathbf{T} \rangle_V$ and $\langle \mathbf{A} \rangle_V$ and can now be expressed by:

$$2W_t = \lambda_{11} \nabla T_1^2 + \lambda_{22} \nabla T_2^2 + \lambda_{33} \nabla T_3^2 + \lambda_{12} \nabla T_1 \nabla T_2 + \lambda_{13} \nabla T_1 \nabla T_3 + \lambda_{23} \nabla T_2 \nabla T_3$$  (4)

with the thermal conductivity tensor and the temperature gradient vector of the composite material defined as:

$$\mathbf{A} = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} \end{pmatrix}$$  (5)

and

$$\nabla \mathbf{T} = ( \nabla T_1 \nabla T_2 \nabla T_3 )^T$$  (6)

3.2. Numerical solving

To find the values of coefficients in the matrix, special situations with different boundary conditions must be built in such a way that for a particular temperature difference only one value in the temperature gradient vector is non-zero and all others become zero. Then the 6 corresponding effective components of the thermal conductivity tensor can be evaluated using the non-zero value in the temperature gradient vector and the calculated averaged value of the pseudo thermal energy $W_t$. A temperature difference is assigned for each node belonging to the boundary of the unit cube (RVE) in order to apply the thermal homogenization technique.

To demonstrate the algorithm, the calculation of a coefficient $\lambda_{ii}$ ($i=1,2,3$) is explained in detail (Figure 10). In this case, the boundary conditions have to be prescribed to the RVE in such a way that, except for the temperature gradient in the $y_i$ direction ($\nabla T_i$), all other components become zero. To avoid temperature variation (fluctuation), the corner point temperature (0, 0, 0) is imposed. The coefficient $\lambda_{ii}$ can finally be obtained with the equation:

$$\lambda_{ii} = \frac{2W_t}{\nabla T_i^2}$$  (7)

For the calculation of the coefficients $\lambda_{ij}$ ($i \neq j$), knowledge of the previous coefficient is required (Figure 11). The temperature gradients in the $y_i$ and $y_j$ directions ($\nabla T_i$ and $\nabla T_j$) are non-zero values and the following equation is used:

$$\lambda_{ij} = \frac{2W_t - \lambda_{ii} (\nabla T_i)^2 - \lambda_{jj} (\nabla T_j)^2}{2 \nabla T_i \nabla T_j}$$  (8)
4. Thermal conductivity measurements

4.1. Thermal conductivity measurements of sunflower pith aggregates

The laser flash method has been used to determine, via thermal diffusivity, the effective thermal conductivity of disk samples of sunflower pith in air. The laser was used to heat up the front face of the cylindrical sample. The absorbed heat diffuses throughout the sample and a liquid-nitrogen-cooled infra-red detector was used to monitor the evolution of the back face temperature. Degiovanni’s method [3], which takes into account heat losses, was used to calculate the thermal diffusivity ($\alpha$) from the analysis of the back face temperature–time behaviour. Assuming the sample behaves as a homogeneous medium, the thermal conductivity is then obtained with the expression:

$$\lambda = \alpha \rho C_p$$

(9)

where $\rho$ is the measured apparent density and $C_p$ is the specific heat of the material obtained from calorimetry experimental data. For a relative humidity of 40% and a temperature of 20°C, the mean value of thermal conductivity of pith samples is close to 0.044 W/(m K).

4.2. Thermal conductivity measurements of sunflower pith packed bed

A thermal constant analyser test system, called Hot Disk, has been used to performed thermal conductivity measurements of sunflower stem packed bed. The method is a transient plane source technique developed by Gustafsson in 1967 [4]. This technique allows to measure the thermal conductivity of a wide range of materials, in the range of 0.005 W/(m K) to 500 W/(m K) over a wide temperature range. To perform the experimental measurements, a cylinder container (40mm in diameter, 80mm in height) with a slit allowing insertion of the hot disk sensor, has been used. The first half of the container is firstly filled with aggregates of sunflower pith. The sensor is then introduced by the thin slit and finally the container is completed with other aggregates. The sensor is thus sandwiched between two thicknesses of grains. Once the assembly is performed, a small constant current is supplied to the sensor, causing a temperature increase. By monitoring this temperature increase over a short period of time, it is possible to obtain accurate informations on the thermal conductivity of the packed bed. Pith particles have, firstly, been sieved to remove particles whose size distribution is over 2.5mm. The apparent thermal conductivity has then been measured for a relative humidity close to 40%, a temperature of 20°C and for four values of volume fraction of air cavities in the packed bed in the range 6.1 - 37.3%. For each air volume fraction, five measurements have been performed. The standard deviation is lower than 0.5%. Graph of Figure 12 in Section 5 shows the mean evolution of the apparent thermal conductivity.
5. Numerical results

DEM computations have been performed with three sizes of pith grains: 1, 1.5 and 2.5mm (Figures 5 and 6). A predetermined penetration length has been imposed or refused between grains to vary the air volume fraction in the packed bed. Once the RVE is cut in the modeled packed bed, the pith thermal conductivity (0.044 W/(mK)) measured with the laser flash technique is attributed to grains and the air thermal conductivity (0.026 W/(mK)) is assigned to the volume surrounding the aggregates. A thermal resistance (0.05 m$^2$K$^{-1}$) has in addition been imposed between each aggregate in contact to model a boundary resistance. Graph of Figure 12 shows the evolution of the effective thermal conductivity with its upper and lower bond of the packed bed for a volume fraction of air between grains in the range 8.0 - 37.1%.

![Figure 12](image.png)

Figure 12. Apparent thermal conductivity values measured with the Hot Disk system and computed with the numerical model.

The thermal conductivity values computed with the numerical model are lower than the measured values. A maximal deviation of 13.8% is obtained for an air volume fraction of 37.1% and a deviation between 9.7 and 14.1% is registered for an air volume fraction of 8.0%. In addition, the trend of the plotted curves are not the same. Whereas the measured thermal conductivity increases with the air volume fraction, the computed thermal conductivity decreases for air volume fraction in the range 22 - 37%. The deviation and the inversion of trend for high air volume fraction can be explained by convective and radiative heat transfer [9, 10] in air cavities surrounding the grains, not taken into account in the numerical model.

The second observation is about the individual thermal conductivity value of pith aggregate. The packed bed sample is made up from pith aggregates taken on all the stem, whereas the laser flash measurements have been performed on disk samples taken in the top of sun flower stem. The presence of air cavities in the other part of the stem doesn’t allow the cutting of homogeneous disk samples. In addition, the residual presence of stem bark in the packed bed can also contribute to a deviation in the thermal conductivity of the aggregates. Uncertainties exists thus in the numerical model but also in the experimental measurements. Indeed, the volume fraction of air cavities is not easy to evaluate due to the scattering in density value of the pith material. To take into account additional thermal pore effects, preliminary calculations with contributions of convection and radiation in the effective thermal conductivity value of air have been performed:

$$\lambda_{\text{air}} = \lambda_{\text{cond}} + \lambda_{\text{conv}} + \lambda_{\text{rad}}$$ (10)

Therefore, according to the works of Litovski and Loeb, the effective thermal conductivity of air has been increased linearly from 0.026 W/(m K) for 8% of air volume fraction up to 0.036 W/(m K) for 37% of air volume fraction. Furthermore the boundary grain thermal resistance has been decreased to a more realistic value of 0.01 m$^2$K$^{-1}$. The computed results are given
in Figure 12. The minimal and maximal deviations are decreased respectively to 3.4 and 4.0%. These obtained overall thermal conductivity values show that contribution of convective and radiative heat transfer in the packed bed have to be considered [11].

6. Conclusions
A combined finite-discrete element method devoted to simulate the compaction of sunflower pith particles in a container and to calculate the effective thermal conductivity of particle packing bed has been formulated using a velocity Verlet algorithm and a homogenization technique. DEM has been used to recreate the actual process for filling a volume element with a high volume fraction of aggregates. By permitting penetration between grains, the maximal volume fraction of aggregates in the final RVE is close to 92%. The developed surface of individual sunflower pith grains has been scanned in 3D to be reconstructed from point sets and finally meshed in 3D. In this way, a grain is composed of a clump of discrete elements located at mesh nodes. To calculate the effective thermal conductivity of the built RVE, thermal conductivity values of pith samples and air have been attributed to the different phases of the RVE. A boundary thermal resistance has in addition been applied between each grain in contact. Finally, a homogenization technique with a uniform temperature gradient at the boundary has been performed. Results of numerical simulations have been compared to experimental values determined for the packed bed of the sunflower pith particles. Whereas the measured thermal conductivity increases with the volume fraction of air between grains, the computed thermal conductivity is slightly reduced for air volume fraction up to 22%. This deviation would be due to convective and radiative heat transfer in the packed bed, not taken into account in the initial numerical model. To confirm this hypothesis, preliminary calculations considering the contribution of convection and radiation have been performed. The results are promising and have to be validated by thermal conductivity measurements of the sunflower aggregates/organic binder biocomposite.

7. References
[1] Bornert M, Bretheau T and Gilormini P 2001 Homogénisation en mécanique des matériaux 1: Matériaux aléatoires élastiques et milieux périodiques. Hermes Sciences Publicat.
[2] Cundall P A 1971 Symposium of the International Society for Rock Mechanics, Nancy, France II 8
[3] Degiovanni A 1977 Thermal diffusivity and flash method Rev Gen Therm 16(185)420-41
[4] Gustafsson S E, Naturf Z 1967 22a1005-11
[5] Hill R 1965 A self-consistent mechanics of composite materials J. Mech. Phys. Solids 13 213-22
[6] Iorga L, Pan Y and Pelegri A 2008 Numerical characterization of material elastic properties for random fiber composites J. Mech. Mat. Struct. 30 1279-98
[7] Jerier J-F, Imbault D, Donze F-V and Doremus P 2009 A geometric algorithm based on tetrahedral meshes to generate a dense polydisperse sphere packing Granular Matter 1143-52
[8] Kanit T, Forest S, Galliet I, Mounoury V and Jeulin D 2003 Determination of the size of the representative volume element for random composites: statistical and numerical approach, Int. J. Solids Struct. 40 3647-79
[9] Litovsky E, Shapiro M and Shavit A 1996 Gas pressure and temperature dependences of thermal conductivity of porous ceramic materials: Part 2, refractories and ceramics with porosity exceeding 30% J. Am. Ceram. Soc. 79 (5)1366-76
[10] Loeb A L 1954 Thermal conductivity: VIII, a theory of thermal conductivity of porous materials J. Am. Ceram. Soc.37 (2)96-99
[11] Magniont C 2010 Contribution la formulation et la caractérisation d’un commatériaux de construction base d’agroressources PhD Thesis. Toulouse III University
[12] Cundall P A and Strack O D L 1979 Geotechnique 29 1
[13] Wang Y and Mora P 2008 Modeling Wing Crack Extension: Implications for the Ingredients of Discrete Element Model Pure and Applied Geophysics 165 (3-4) 609-20
[14] Widom B 1966 Random sequential addition of hard spheres to a volume J. Chem. Phys. 44 3888-94
[15] Swope W C, Andersen H C, Berens P H, Wilson K R 1982 A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters The Journal of Chemical Physics 76 (1)