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Thermal Behavior of Clay-Based Building Materials: A Numerical Study Using Microstructural Modeling

Ahmed Lkouen[1*], Mohamed Lamrani[2], Ahmed Meskini[1], Abdelhamid Khabbazi[3]

[1]LM2I, ENSEM, Hassan II University, Casablanca, Morocco
[2]LGCEM, EST Sale, Mohamed V University, Rabat, Morocco
[3]EMDD_CERNE2D, EST Sale, Mohammed V University, Rabat, Morocco
Email: *a.lkouen@gmail.com

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Abstract

A large part of the energy savings in the building sector comes from the choice of materials used and their structures. We are interested, through a numerical study, in establishing the link between the thermal performance of composite materials and their microstructures. The work begins with the generation of a two-phase 3D composite structure, the application of the Random Sequential Addition (RSA) algorithm, and then the finite element method (FE) is used to evaluate, in steady-state, the effective thermal conductivity of these composites. The result of the effective thermal conductivity of composite building material based on clay and olive waste at a volume fraction of 10% obtained by simulation is 0.573 $W \cdot m^{-1} \cdot K^{-1}$, this result differs by 3.6% from the value measured experimentally using modern metrology methods. The calculated value is also compared to those of existing analytical models in the literature. It can be noticed also that the effective thermal conductivity is not only related to the volume fraction of the inclusions but also to other parameters such as the shape of the inclusions and their distribution. The small difference between the numerical and experimental thermal conductivity results shows the performance of the code used and its validation for random heterogeneous materials. The homogenization technique remains a reliable way of evaluating the effective thermal properties of clay-based building materials and exploring new composite material designs.

Keywords

Effective Thermal Conductivity, Finite Element Calculation, Homogenization, RSA, Composite

1. Introduction

In the building sector, Morocco has put in place a legislative framework that sets out the rules for the energy performance of buildings, namely Law 47-09 on energy efficiency and the Thermal Building Regulations in Morocco. In this context, particular importance is attached to improving the living conditions of the inhabitants of the Draa-Tafilalet region, which is geographically located in the south-eastern part of Morocco, and characterized by a dry climate (the temperature varies between −1˚C and −7˚C in winter and can reach more than 48˚C in summer. [1]), by improving the quality of thermal insulation of the clay-based materials historically used in this region. Some research [2] [3] has been carried out to improve the thermal behavior of clay by combining it with additives of animal [4] or vegetable [5] origin. Several parameters influence the thermal properties of composite materials (e.g. the volume fraction of inclusions, their shape, property contrast, dispersion, and orientation of additives). Homogenization techniques aim to take into account information on the microstructure of materials in order to calculate their effective properties based on the laws of behavior at the scale of a representative elementary volume [6]. The steps of this technique are shown in **Figure 1**. the first step consists in generating a 3D microstructure with randomly oriented and dispersed additives, then boundary conditions are applied and the response of the volume is computed using numerical techniques such as the Finite Element (FE) [7] [8]. M. Wang *et al.* [9] have developed a random generation-growth method and they used the Lattice Boltzmann method to Modeling and predicting the effective thermal conductivity of random open-cell porous foams. We propose here a random generation method with ellipsoidal inclusions at different aspect ratios. Then a statistical mean on the results obtained by the finite element method allows for evaluating the thermal conductivity of building material based on clay and olive waste.

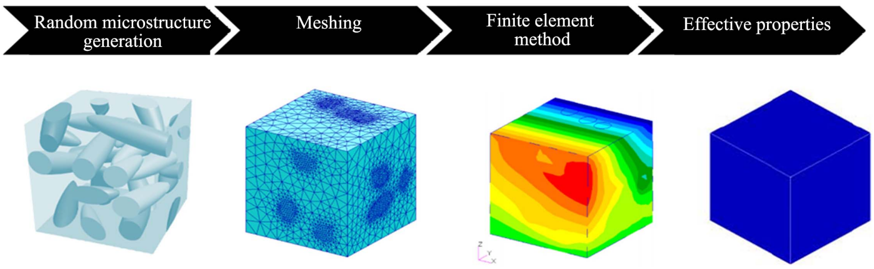


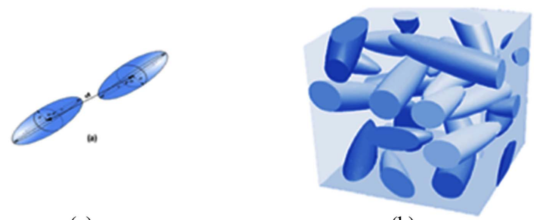
Figure 1. Numerical homogenization process [10].

2. Random Microstructure Generation Methods

In this section, the composite material studied is represented by a geometry of the granular structure in which the distribution requires a probabilistic approach. Ellipsoidal particles are created with a free choice of the orthogonal distances of the ellipsoid (a, b, c), then the coordinates of their center and the Euler angles (Ψ, θ, φ), which define the rotation of the ellipse, are generated randomly in a cubic matrix of volume $V = L^3$, using the Random Sequential Adsorption algorithm RSA developed under Matlab. The particles are randomly introduced one after the other until the desired volume fraction is obtained, while checking the following conditions:

If a new particle overlaps previously placed particle(s), then this attempt is rejected. Otherwise, the placement is accepted. The distance *d* between the centers of the ellipsoids must be greater than the largest of the orthogonal distances (a, b, c) (Figure 2(a)).

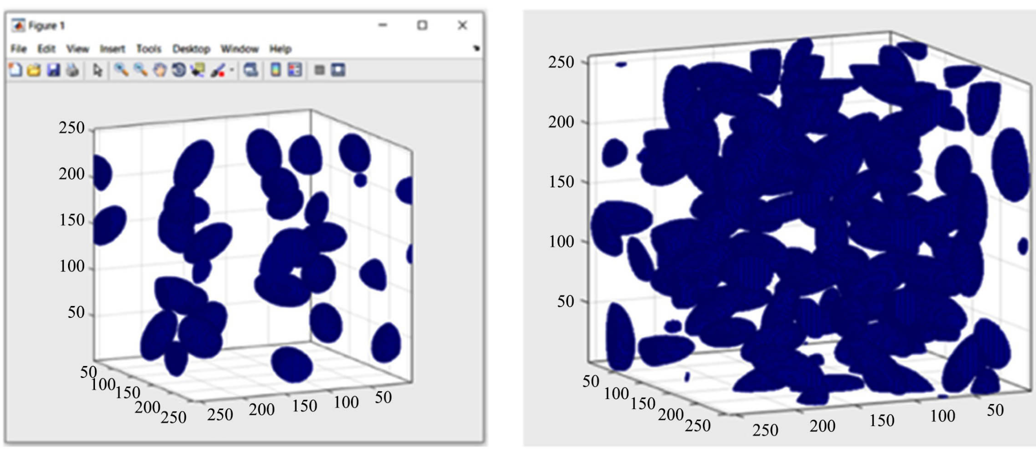
If the particle intersects a face of the matrix it will be extended by the opposite face to ensure the periodicity of the macroscopic material (Figure 2(b)).



(a) (b)

Figure 2. (a) Parametrization of ellipsoidal particle and no overlap condition; (b) periodization of the 3D microstructure.

Figure 3 shows two examples of samples generated by the RSA algorithm: Structure S_1 (Figure 3(a)) and structure S_2 (Figure 3(b)) with respectively 5% and 20% volume fraction additives. The orthogonal distances (a, b, c) of the ellipsoid have been chosen to have an aspect ratio of 4:2:3. The edge of the cubic structures is expressed in 10^{-2} cm.



(a) (b)

Figure 3. Examples of structures generated by RSA algorithm: (a) structure S_1 with a volume fraction of 5%, Number of particles: 23. And (b) structure S_2 with a volume fraction of 20%, Number of particles: 90.

3. Calculating the Effective Thermal Conductivity of the Composite Using Finite Element

3.1. Material and Microstructure

We have studied the composite consisting of clay reinforced with a 10% volume fraction of olive waste, which is modeled by ellipsoids with an aspect ratio of 4:2:3, randomly oriented, and dispersed in a clay matrix. An example of this structure with 78 particles is shown in **Figure 4**. Thermal contact between the clay and olive waste is assumed to be perfect. The conductivities of the composite constituents are:

$\lambda_{Clay} = 0.651\ \mathrm{W \cdot m^{-1} \cdot K^{-1}}$ and $\lambda_{OW} = 0.099\ \mathrm{W \cdot m^{-1} \cdot K^{-1}}$. These taken values are those of clay and olive waste from the Draa Tafilalt region.

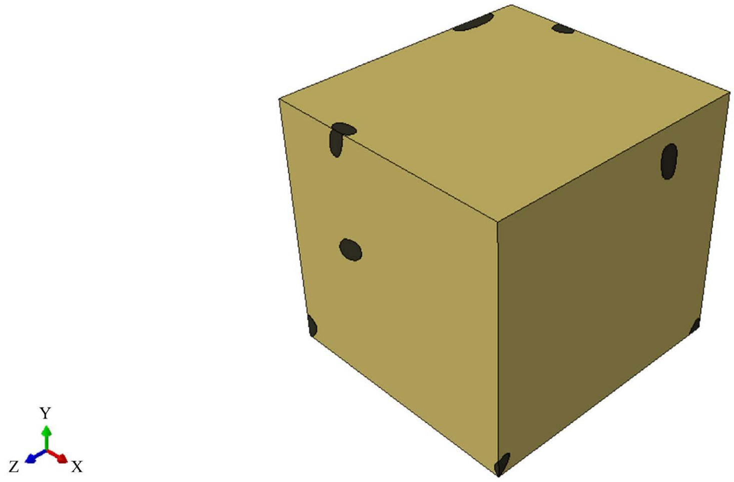


Figure 4. Example of a structure generated by the RSA algorithm with a 10% volume fraction.

Each generated structure is then transferred to the ABAQUS software to perform a finite element calculation of the effective thermal conductivity of the studied composite

3.2. Numerical Model of Heat Transfer

To study the thermal properties, an external temperature gradient is applied then the heat equation is solved.

- Laplace's Equation: The effective thermal conductivity, in steady-state, can be obtained from the thermal conductivities of the matrix and the inclusions by solving the following Laplace equation [11]:

$$div\left(\lambda(\boldsymbol{r})\,\boldsymbol{grad}\,T(\boldsymbol{r})\right) = 0 \tag{1}$$

with $\lambda(\boldsymbol{r})$ is the local thermal conductivity and $T(\boldsymbol{r})$ local temperature.

- Heat flux conservation: Partial differential equations lead to the physical notion of conservative flow given by a gradient:

$$\iiint div\left(\lambda(\boldsymbol{r})\,\boldsymbol{grad}T(\boldsymbol{r})\right)\mathrm{d}V = 0 \tag{2}$$

Using the divergence-flux formula (Ostrogradsky's theorem), it comes:

$$\oiint \lambda(\boldsymbol{r})\,\boldsymbol{grad}T(\boldsymbol{r})\cdot \mathrm{d}\boldsymbol{s} = 0 \tag{3}$$

we deduce from this:

$$\oiint \boldsymbol{j}_{th}(\boldsymbol{r})\cdot \mathrm{d}\boldsymbol{s} = 0 \tag{4}$$

To simplify the resolution of Equation (1), unidirectional heat flux is imposed. But since the particles are randomly distributed and oriented, the material is isotropic at full scale, while the individual realizations are not necessarily isotropic, which requires calculating an average value over the different directions with an acceptable percentage of error in isotropy.

The effective thermal conductivity in the x-direction, for example, can be obtained by the relationship:

$$\frac{\lambda_{eff,x} * \Delta T}{L} * S = \iint -\lambda \left(\frac{\mathrm{d}T}{\mathrm{d}x} \right) \mathrm{d}y\mathrm{d}z \tag{5}$$

A statistical approach on a representative number of realizations, based on the methodology of Kanit *et al.* [6], is used to estimate the effective thermal conductivity with a given precision.

3.3. Boundary Conditions

A temperature gradient is imposed between two opposite sides, in a stationary state, which generates a heat flux directed towards low temperatures. we have chosen to work in a unidirectional model, so the sides normal to the heat flow are insulated. The boundary conditions are shown schematically in **Figure 5** and are given by the following equations:

$$\begin{cases} T(x=0) = 295\ \mathrm{K} \\ T(x=L) = 273\ \mathrm{K} \end{cases} \tag{6}$$

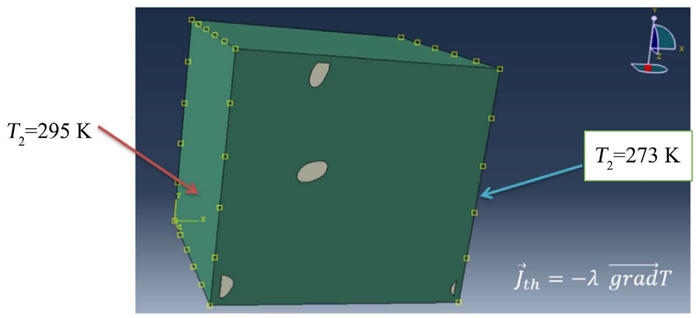


Figure 5. Boundary conditions.

3.4. Meshing

The RVE (Representative Volume Element) geometry created in the previous section has meshed in order to determine the thermal properties of the composite material. A free meshing with tetrahedral elements leads generally to a fairly high density of elements at the matrix/inclusion interface and it can be easily automated. It is used to obtain a high-quality periodic discretization of matrix-inclusion microstructures with as few elements as possible (**Figure 6**). 173,544 elements have been generated using 10-node tetrahedron elements. The optimal meshing parameters have been chosen on the basis on the conservation of the topology of the interfaces of the microstructure.

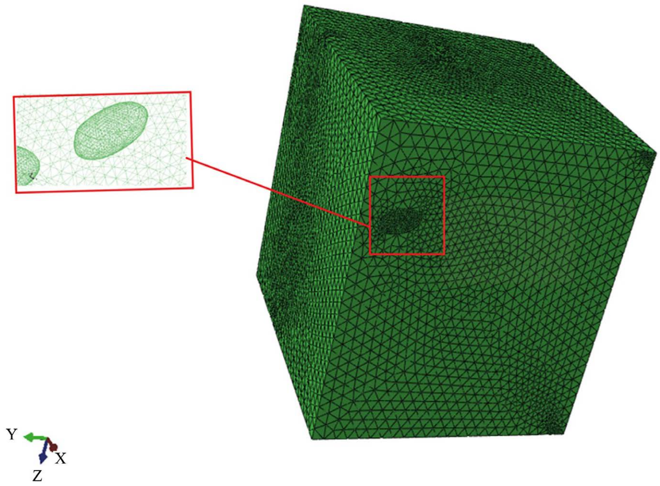


Figure 6. Volume mesh of an RVE with a volume fraction of 10%.

4. Results and Discussion

4.1. Heat Flux

The thermal conduction inside the material is governed by Fourier's law. The heat flux obtained within the elementary volume is almost uniform as shown in Figure 7, which is in accordance with the stationary regime established, except in the surroundings of the inclusions where variations in heat flow are observed, this is clearly shown on the curve of heat flow variations given by Figure 8. These fluctuations in heat flow at the matrix/inclusion interfaces can be explained by the difference in thermal conductivities of the two constituents of the composite material. We obtain, on average, a thermal flux in the order of 0.05355 $W \cdot m^{-2}$.

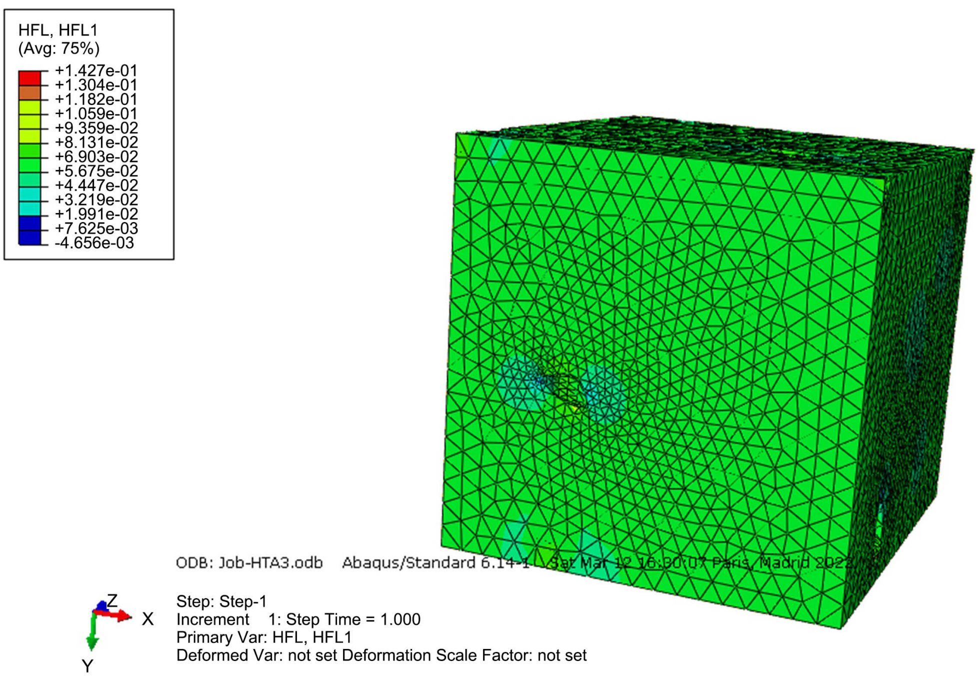


Figure 7. Heat flux along the temperature gradient.

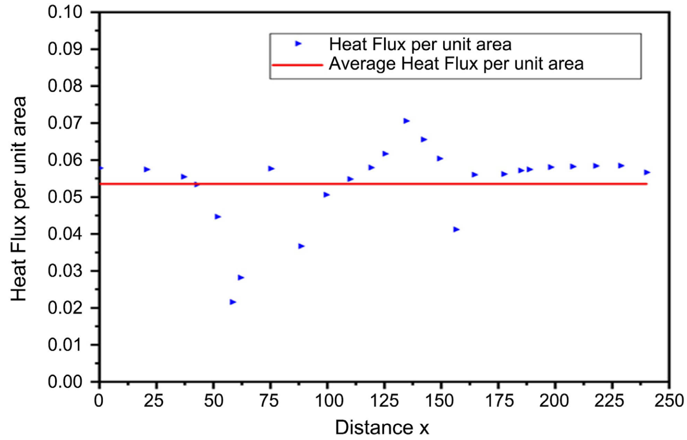


Figure 8. Heat flow variations within the material along the temperature gradient.

4.2. Temperature Distribution

For illustration, an example of temperature distribution within the elementary volume (Figure 9) shows a unidirectional decrease along the x-axis. It also appears that the planar aspect of the isothermal surfaces is modified in the proximity of the additives. In effect, the temperature field is not uniform over a section perpendicular to the direction of the heat flow. This reflects the opposition of grains to heat transfer due to their low thermal conductivity making the material more insulating.

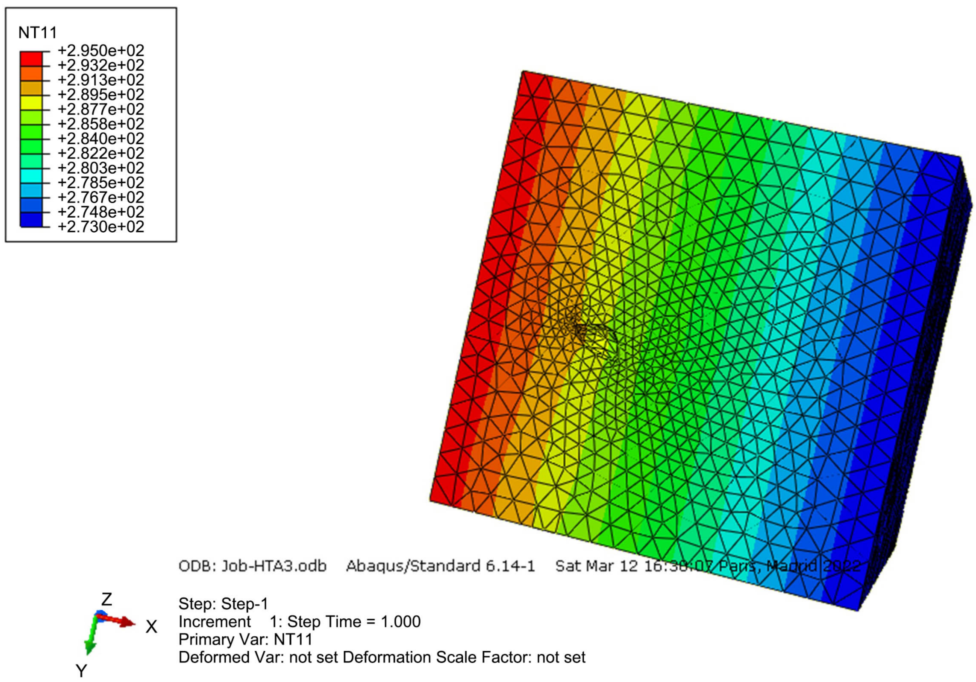


Figure 9. Temperature distribution.

An example of the result of temperature variations in the direction of thermal diffusion is shown in Figure 10. The equation of the linear regression makes it possible to go back to the value of the thermal conductivity.

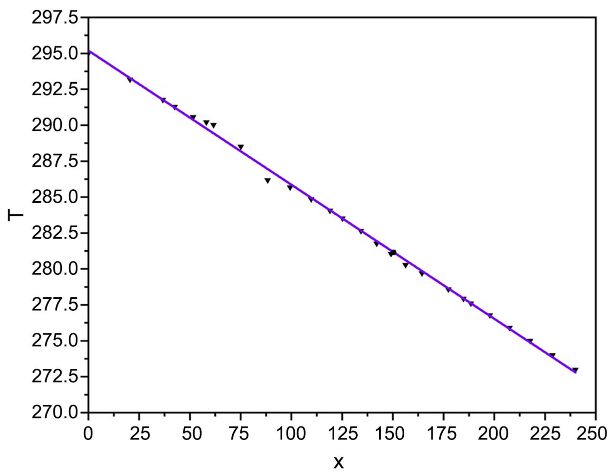


Figure 10. Temperature variation along the diffusion direction.

4.3. Effective Thermal Conductivity

Many geometrical realizations (several random draws of positions and orientations) for the same 3D microstructure (same volume fraction and aspect ratio) were simulated. Then the statistical average and the relative deviation were calculated for each number of implementations. The increase in the number of realizations was stopped when there is the convergence of the thermal conductivity. the average thermal conductivity and its dispersion calculated are given in Figure 11. The variance of computed apparent properties for each number of realizations is used to define the precision of the estimation, which corresponds to an uncertainty of less than 0.5% in our case.

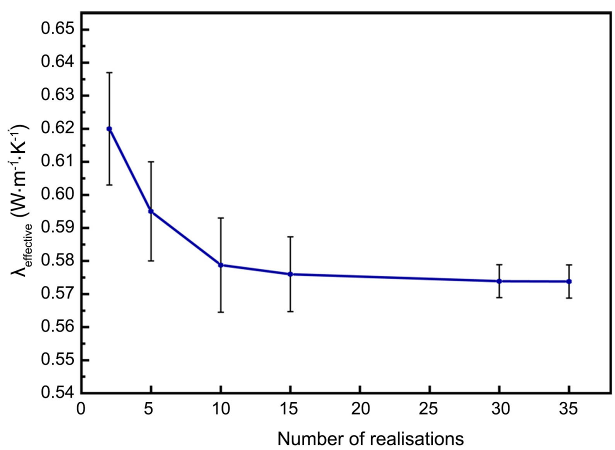


Figure 11. Average values and confidence intervals on average of thermal conductivity as a function of the number of realizations.

The same composite material has already been studied experimentally and its thermophysical properties have been characterized using modern metrology methods [12].

Figure 12(a) represents the prepared sample of the clay material reinforced with a volume fraction of 10% olive waste, the preparation was carried out in the laboratory LEME (in High school of technology – Sale). The characterization of the thermal conductivity of the sample was carried out by the method of the asymmetric hot plate in steady-state whose modeling is presented in **Figure 12(b)**. On average, the experimentally measured thermal conductivity is: $\lambda_{exp} = 0.553\ \mathrm{W \cdot m^{-1} \cdot K^{-1}}$

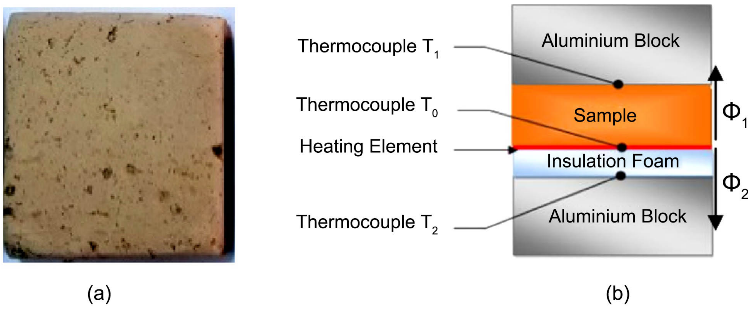


Figure 12. (a) Clay-olive waste sample; (b) Experimental device of the asymmetric hot plate method.

The calculated value of the equivalent thermal conductivity is also compared to those obtained by the different analytical models existing in the literature.

The expressions of the equivalent thermal conductivity for each model are given by the following relationships [13] [14] [15]:

- Series model:

$$\lambda_{Series} = \frac{1}{\frac{1-y}{\lambda_{Clay}} + \frac{y}{\lambda_{O.w}}} \tag{7}$$

- Parallel model:

$$\lambda_{parallel} = (1-y)\lambda_{Clay} + y\lambda_{O.w} \tag{8}$$

- Beck model:

$$\lambda_{Beck} = \sqrt{\lambda_{series} \cdot \lambda_{parallel}} \tag{9}$$

- Maxwell model:

$$\lambda_{Maxwell} = \frac{(1-y)\lambda_{Clay}\left(2\lambda_{Clay} + \lambda_{O.w}\right) + 3y\lambda_{Clay}\lambda_{O.w}}{(1-y)\left(2\lambda_{Clay} + \lambda_{O.w}\right) + 3y\lambda_{Clay}} \tag{10}$$

- Woodside model:

$$\lambda_{woodside} = \lambda_{O.w}^{y} \cdot \lambda_{Clay}^{(1-y)} \tag{11}$$

with:

y and $\lambda_{O.w}$ are respectively the volume content and the thermal conductivity of olive waste and λ_{Clay} is the thermal conductivity of the continuous phase (clay).

Table 1 gives the numerical and experimental results as well as the values from the analytical models and also the relative deviations from the experimental value.

Table 1. Comparison of experimental, numerical and analytical thermal conductivity values.

	Experimantal value ($W \cdot m^{-1} \cdot K^{-1}$)	Simulated value ($W \cdot m^{-1} \cdot K^{-1}$)	Analytical model values ($W \cdot m^{-1} \cdot K^{-1}$)				
			Series	Beck	Woodside	Maxwell	Parallel
Thermal conductivity	0.553	0.573	0.418	0.499	0.593	0.577	0.596
Relative deviation	…	3.6 %	24.4%	5.4%	2.5%	4.3%	7.7%

The small difference between the numerical and experimental results shows the performance of the computational code used and its validation for random heterogeneous materials, and it appears that the Woodside geometric model is the closest to represent this sample, which reflects the geometric mean of the random distributions of additives in the clay matrix.

5. Conclusions and Perspectives

In this work, a numerical finite-element-based methodology is presented for predicting the effective thermal conductivity of random heterogeneous materials. The study was particularly interested in a clay-based building material from the Draa Tafilalt region (southern Morocco) that is characterized by a dry climate, with rapid daily temperature variations, which requires the effect of heat stress on these materials will be studied as a continuation of this work.

Compared to existing models and experimental results, this method is very promising as a tool to predict the effective properties of clay-based composites, and also the design of new ones used to increase the energy efficiency of buildings. The 3.6% deviation observed from the value found experimentally can be explained by the fact that the particles of olive waste that were inserted in the clay during the experimental preparation of the samples do not have the same aspect ratio. In perspective, we will propose the generation of 3D structures with random distributions and orientations of inclusions having non-identical sizes.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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