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# Numerical investigation of porous materials composites reinforced with natural fibers

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**Abstract.** The present article tends to predict the effective thermal properties of porous biocomposites materials. The composites matrix consists on porous materials namely gypsum and the reinforcement is a natural fiber as date palm fibers. The numerical study is done using Comsol software resolving the heat transfer equation. The results are fitted with theoretical model and experimental results. The results of this study indicate that the porosity has an effect on the Effective thermal conductivity biocompoites.

**Nomenclature**

$k_f$ : thermal conductivity of fibers,
$K_m$ : thermal conductivity of matrix
ETC : effective thermal conductivity $(W.m^{-1}.K^{-1})$
$DPF_3$ : date palm fibers of 3mm length
$DPF_6$ : date palm fibers of 6mm length
$V_c$: composite volume
$V_{ce}$ : elementary cell volume
x, y, z : elementary cell dimensions
X, Y, Z : biocomposite dimensions
r : fiber radius, L : fiber length

## 1. Introduction

Reducing the energy consumption in building is a current major problem which interests a several researchers [1, 2]. Among solutions to resolve this problem is the using material which deals with thermal insulation [3-5]. The use of biomaterials containing natural fibers as a reinforcement becoming a necessity considering their numerous advantages such as the combination of good mechanical, thermal, and acoustic properties those allow these types of materials to be used for different applications [6, 7].
Generally, the introduction of NF induces a porous material. The recourse to the porous material and composites is justified by the fact that they present the advantage of lower heat conduction and a high strength. The parameters such as pore size, porosity and pore distribution, particle size and particle distribution make the heat conduction in the porous material and composites very complicated to predict [8].
The effective thermal conductivity (ETC) is very important to define the insulation materials degree because thermal expansion by disordered temperature distribution and temperature gradient causes stress concentration around pore and composite. The conventional models for heat transfer in porous material and composite are not perfectly adequate because they are simplified [9-11].

The theoretical modeling of (ETC) of the composite is a very difficult task and requires knowledge of numerous parameters which are sometimes difficult to obtain (parameters related to microstructure, thermal contact resistance, etc.) [12, 13]. Other work on mathematical modeling, experimental characterization on a microscopic scale, and Microstructural analysis can improve the model predicting of the properties of composite materials. Therefore, it can be noted that, no theoretical model is complete to predict the thermal conductivity of Composites with precision, which makes numerical simulation indispensable for validating theoretical models.
Several models have been proposed for modeling and predicting the effective thermal conductivity of porous materials. Yue *et al* [14] used the face centered cubic model (FCC) to predict the ETC of the polymer matrix reinforced by metallic fillers. Chikhi *et al* [9] studied also the reinforcement of polymer materials with metallic fillers in aim to increase the ETC of composites. The results show that at high concentration of fillers, the numerical model diverges to the experimental and theoretical model results. This trend may be due to the resistance contact in the composites. Asakuma [8] investigated the factors that determine the effective thermal conductivity of porous structures and composites, by the homogenization method. Calmidi et al. [15] presented a one-dimensional thermal conduction model by considering the porous structure as a two-dimensional. Djoudi *et al*. [16] investigated the ETC of DPF reinforced gypsum materials, using auto-coherent homogenization method. They concluded that this method gives a good results for small fraction of fibers (>2*%w*).
The experimental used techniques and the modeling approach are based on the fact that the adobe is clearly a bio-composite material [17]. The composite material in which the matrix is the wet soil and the filler is a set of tubular straws. The simulations of thermal effective property were performed using COMSOL™ software. The main aim of this paper is to investigate numerically the ETC of biocomposite material based on gypsum material reinforced with DPF. The simulations are performed using Comsol Multyphysics software in stationary stat. The numerical results of this work are validated with theoretical models of predicting ETC and experimental results obtained previously [3].

## 2. Materials process
The table 1 illustrates the thermophysical properties of different materials used in this study. The thermophysical properties of the biocomposite based on gypsum reinforced on date palm fibers (DPF) were determined experimentally using the Ct-meter Apparatus. The detail of the experimentation process is given in previous work [3].

**Table 1.** Thermal properties of materials used in the simulation

| Thermophysical properties | *k* ($W.m^{-1}.K^{-1}$) | ρ ($Kg.m^{-3}$) | Cp (J/kg.K) |
|---|---|---|---|
| Gypsum | 0.44 | 1130 | 1400 |
| DPF | 0.085 | 388 | 930 |
| Air | 0.025 | 1.225 | 0.34 |

### *2.1. Theoretical models to predict thermal conductivity*
Regarding the literature several models have been proposed to predict the thermal conductivity of fiber-filled composites in aim to fit experimental and numerical data with various models [18]. Theoretical models used in this study are: Parallel and series models, Maxwell, Hatta and Taya, Hashin and Shtrikman models [9].

### *2.2. Descriptive of modeling with COMSOL software*

In order to model the transfer within the composite, we consider an elementary cell corresponding to a fiber considered a cylindrical shape (l, r) centered in a parallelepiped (PL) matrix Figure 1. The temperature field in the composite material is defined by solving numerically the Laplace equation using a finite element formulation with the following boundary conditions. The two faces perpendicular to the direction of the heat flow are isothermal at temperatures of $T_1$ and $T_2$ respectively. The faces parallel to the direction of the heat flow are adiabatic. The transfers by radiation and convection are negligible; the thermal contact resistance between matrices and charges is negligible; the dispersion of the fibers in the matrices is homogeneous;

#### *2.2.1. Modeling without porosity account*

The Figure 1 presents the elementary cell with limit conditions.

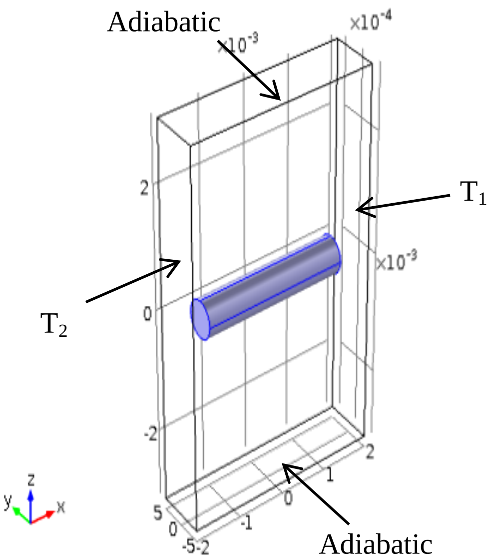


**Figure 1.** Elementary cell with limit

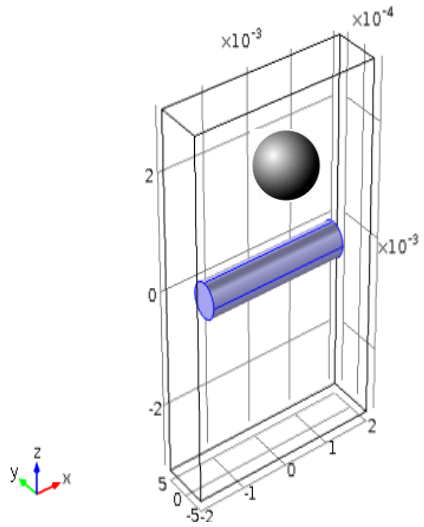

**Figure 2.** Elementary cell with pores

The heat flux that passes through the hot face towards the cold face is calculated from the integration of the Laplace equation (equation 1) applied to the boundaries of the elementary cell of the composite on the y direction.

$$Q = \int_A k \frac{\partial T}{\partial y} dxdz \quad (1)$$

With: Q is the heat flux, and *k* the effective ther mal conductivity of the biocomposite.
*x* et *z* present the surface exchange.
To simplify the problem and minimize computation time, some assumptions are used:

$$V_c = X * Y * Z \quad (2)$$
$$V_{ce} = x * y * z \quad (3)$$
$$V_f = L * 2\pi r^2 \quad (4)$$
$$V_{ce} = V_{comp}/N \quad (5)$$

With:
L: the fiber length; r: the fiber radius and N the fibers number in the biocomposite ;
Taken into a count that the fiber is included in the gypsum (x>L; y>r; z>r).

$$k_{eff} = \frac{Q}{A} \frac{L_y}{(T_1 - T_2)} \quad (6)$$

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Where the surface exchange A= x × z (m²); y is calculated, $\Delta T = T_1 - T_2$ (°K) is the temperature variation. The effective thermal conductivity is calculated using the Eq. 7.

$$k_{eff} = (Q * y)/(x * z * (T_1 - T_2)) \quad (7)$$

*2.2.2. Modeling with porosity account*

For the case of the simulation taken into account the void, the presence of the void in the biocomposites is mentioned as a sphere of radius R. The thermal properties of the void are similar to the air properties mentioned below. The Figure 2 presents the elementary cell with void.

## 3. Results and discussions

The main objective of this work is to investigate the void effect on the thermal conductivity of the composites

*3.1. Modelization results without porosity account*

The Figure 3 Presents the results comparison between numerical and theoretical models with the experimental results of the effective thermal conductivity of biocomposites reinforced with fibers of 3mm and 6mm.

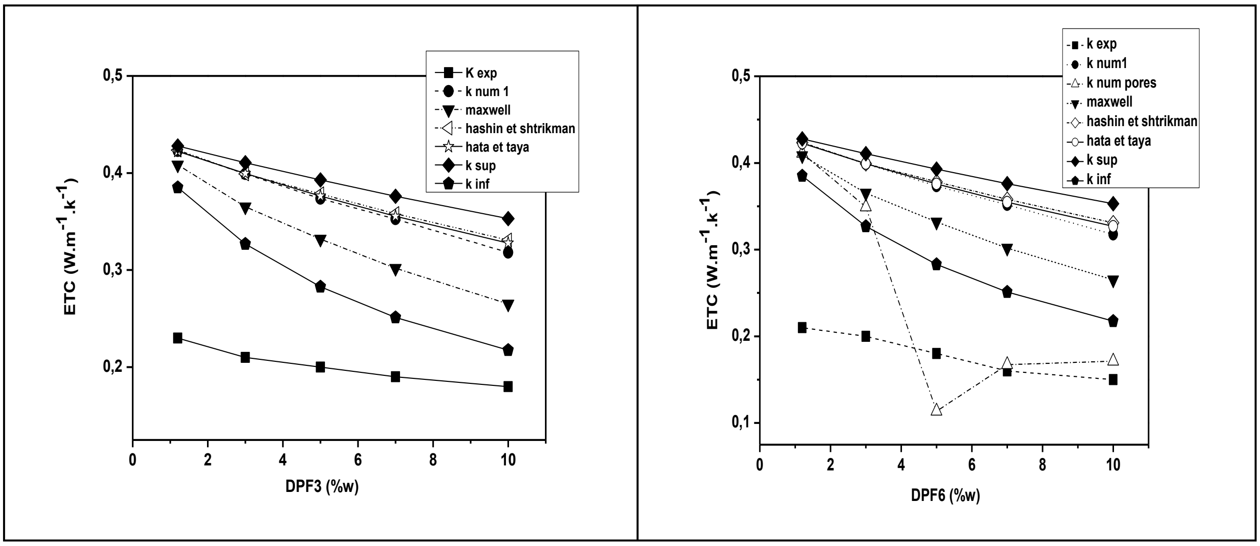


**Figure 3.** Comparison of thermal conductivities results of biocomposites; a) $DPF_3$; b) $DPF_6$

It can be seen from Figure 3, that the increase of the fiber mass concentration induces a non-linear decrease of the effective thermal conductivity of biocomposites reinforced with DPF length of 3 and 6 mm. This decrease is mainly due to the relatively low thermal conductivity of the inclusions (date palm fibers) compared to the matrix (gypsum) one. A similar behavior has been reported in the work of Djoudi et al. [16] who studied numerically the effect of the addition of date palm fibers on the thermal properties of gypsum concrete using the self-coherent homogenization method. The results showed that the effective thermal conductivity of the composite decreases as a function of the fraction of the fillers (date palm fibers). Several authors report this result using natural fibers as reinforcement of composites [1, 16]. An opposite trend is reported by Chikhi et al [9] who shows that the *k* of polymer based composite increases increasing the % of the fillers, which indicates that the effective thermal conductivity depends on the thermal conductivity of the inclusions [5, 9].

Comparing the numerical results with the theoretical models prediction of $k_{eff}$, it is observed that for the numerical values of the effective thermal conductivity are included between the lower and upper limits. It is noted that the Maxwell model does not predict the correctly the numerical results of effective thermal conductivity. This result may be due to the fact that the Maxwell model is based only on the thermal conductivities of the constituents, charge and matrix. While, the models Hashin and Shtrikman and Hata and Taya present a good estimation. This is related to the fact that these models introduce parameters related to the inclusions geometry. It should be noted that the Hashin and Shtrikman model agree with numerical results for fiber mass concentrations up to 10%. A low error of 4% at 10%*w* of fibers is recorded for $HG/DPF_3$ and 3% for $HG/DPF_6$. This result shows that the model of Hashin and Shtrikman predicts the $k_{num}$ without voids. Moreover, the model of Hata and Taya is the model that gives the best estimate of the effective thermal conductivity of our bio-composite compared to the other predictions given by the other theoretical models. It should be noted that this model is based not only on the thermal conductivity of the inclusions but also on parameters related to the geometry of the fibers as in our case, short fibers oriented randomly. For comparison with experimental results, the both numerical and theoretical models results diverge. This result demonstrates that an important parameter is not taken into account in numerical and theoretical models. Since the matrix and fibers used in this study are porous materials, it is imperative to introduce the void parameter in the numerical calculations. As known the porosity effect strongly the thermal properties of biocomposites [17]. The next part of this study will take into account the porosity parameter.

### *3.2. Results of modeling with porosity account*

In this section, the numerical study taken into account the presence of voids in bio-composite based on gypsum reinforced with DPF. Figure 4 presents a comparison between the numerical and experimental results as a function of the weight fraction of 3mm and 6mm fibers length

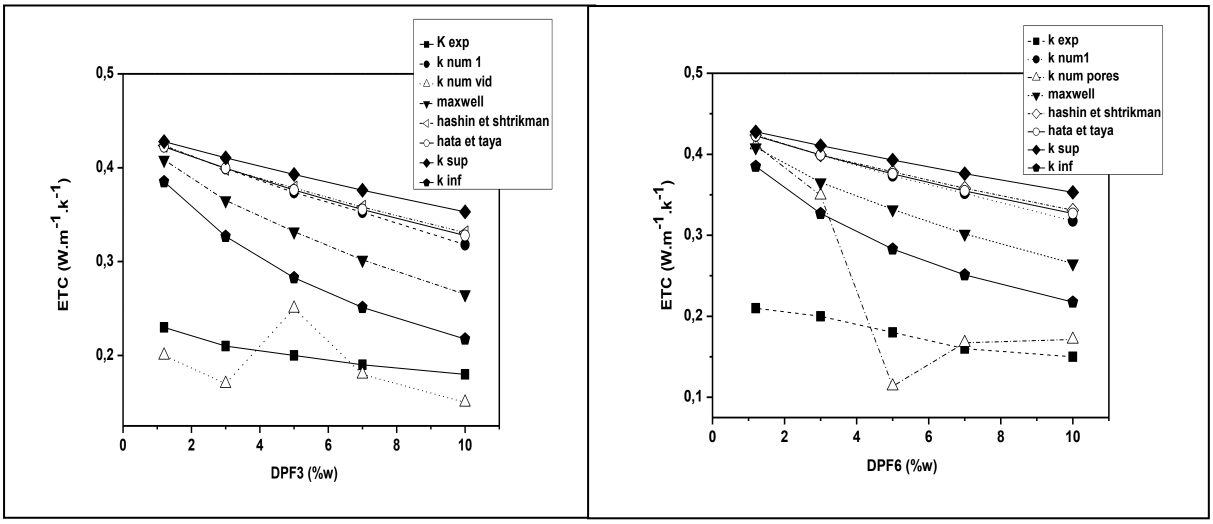


**Figure 4.** Effective thermal conductivity with voids; a) DPF 3mm, b) DPF 6 mm.

It is observed from Figure 4a, that the numerical results are close to the experimental values with an estimated error of 14% except for the concentration of 5%*wt* of DPF with a considerable value. This result may be the consequence of fibers distribution in gypsum.

In addition to the void parameter, the calculated error is mainly affect firstly, by the contact resistances between fiber/fiber and fiber/matrix. Secondly, because in reality when the fiber fraction increases the interaction between fibers increases, hence the formation of a chain of thermal conduction of the fibers which results in an increase in the thermal conductivity of the bio-composite. These two phenomena are not taken into account in numerical modeling which assumes a homogeneous distribution of the fibers in the matrix [9, 14].

Figure 4b indicates that the numerical results of the thermal conductivity in the second diverge from the values obtained by the theoretical models or beyond the 3% concentration of the fibers by 6 mm. This behavior is justified by the fact that theoretical models do not take into account the porosity parameter existing in the constitutions of bio-composites. This result is in line with the result works of [19] which indicates that the porosity effect the ETC of composite material.

## 4. Conclusion

In this study, the ETC of the gypsum matrix loaded with date palm fibers was studied numerically. The finite element method using Comsol Multypysics software was established to estimate the ETC of bio-composites studied in this work. On the one hand, the numerical results are in line with theoretical models results and diverge to the experimental ones for the case that the porosity does not taken into account. On other hand, the simulation taken into account pores of biocomposites, presents a good correlation with experimental results and diverge from the theoretical ones. This trend is due to the fact that the theoretical models do not considering several parameters which affect the ETC, as porosity, orientation morphology of fillers. The fibers size has an important effect on the ETC of biocomposites.

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