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ALGORITHM OF PORES DISTRIBUTION MODEL FOR ANALYSIS AND MEASUREMENT OF THERMAL CONDUCTIVITY OF POLYPROPYLENE POROUS MATERIAL

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ABSTRACT

In the current study, algorithm pore distribution models of porous material are developed for insulator application through establishing the effects of pore shape, content and size, which acts as an expression of the nature of porous material. The arrangement of pore distribution in the polypropylene (PP) system is determined by various irregular shape studies. The model is simulated through representative volume elements (RVEs) with the pore content, which is set in the range of 5–24 vol.%, while the pore sizes are used around 0.2, 2 and 3 μm of diameter size. A significant improvement in the optimization of the insulator model is showed by synergistic effect on decreasing thermal conductivity in increasing the content of the pores. The results obtained show that the various irregular shapes of porous material produce various final results in thermal conductivity. The thermal conductivity of the porous material that contained 24 vol.% of pores significantly improved from 0.22 W/m.K to 0.158 W/m.K. Comparison of the simulation showed that the data matched well with the Maxwell-Eucken and Hashin–Shtrikman bounds models.

Keywords: Finite element analysis; Polypropylene; Porous material; Representative volume elements; Thermal conductivity

1. INTRODUCTION

Thermal management requires materials with known thermal conductivity characteristics to apply to the devices while operational isolation can maintain the temperature. Thermal conductivity is one of the paramount parameters in isolation materials application. Polymer materials, usually applied as insulators, due to their thermal conductivity properties, are known as having lower conductivity. The polymer characteristics in thermal properties presents very low conductivity ranging from 0.1 W/(m K) to 0.5 W/(m K) (Li et al., 2016). In engineering applications, polypropylene (PP) shows good performance in terms of its mechanical properties (Kozderka et al., 2016) and ultraviolet resistance (Li et al., 2015) and it can be processed well. Material PP is categorized as the thermoplastic polymer that can be simply applied in various products based on functional and structural applications. The thermal conductivity of PP is only around 0.22 W/(m.K); it is suitable for isolation field applications. Thus, the thermal conductivity of PP needs improvement to reduce the thermal conductivity. The thermal

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conductivity improvement for insulator applications should satisfy the PP material in lightweight appllications, while being attached to the device. In order to allow for improvement, a new-technique such as the proposed foam material with specific patterns for the shape, size, and structural design of the pores can be considered. In actual data, the polymer foam reported has good results in reducing the weight, due to low density, and good thermal performance, due to heat transfer reduction (Khdir et al., 2015; Suh et al., 2016; Yang et al., 2016). A new method to improve material properties has been proposed by the combination of materials, such as metallic foam and polymer. Several researchers have proposed which various embedded fillers to increase thermal performance (Patti et al., 2016; Wu et al., 2006; Chen et al., 2009). They found a linear increase in thermal diffusivity of high-density polyethylene-based composites.

Realizing that the design of pores construction is critical in determining several properties, such as thermal, mechanical and electrical, the modeling of foam pore structure design is one solution, which has become attractive and effective. Mills et al. (2009) designed a foam pore structure, based on regular Kelvin models with all the material in uniform thickness faces, to predict the compressive impact response of low-density, closed-pore polyethylene and polystyrene foams. Furthermore, based on a three-dimensional (3D) structural modeling, Su et al. (2016) designed microscopic structural models of aluminum (Al) metallic foam and Metal-Porous-Polymer-Composite (MPPCs) with spherical pores and Kelvin's pores, which are established in the finite element code.

There are several techniques to develop the porous model using various shapes and random distribution that can be considered for thermal applications. Khan and Straatman (2016) developed the porous model by using randomly packed sphere shapes for turbulent heat and mass transfer in industrial and food storage applications. In the random 2D structure the multiple relaxation time (MRT)-lattice Boltzmann model has been developed for flow and heat transfer applications (Yang et al., 2016). The work was investigated based on permeability and the Nusselt number, which considered the effect of the disorganized porous structure, while parameters of porosity value ε and effective diameter Den were set as equivalent. Reichenberger et al. (2017) investigated porous materials for use as thermal-neutron detectors. The random geometry of porous materials has been developed using the Monte Carlo method for simulation efforts. The simulation demonstrated the thermal-neutron detection efficiency in certain conditions. Suh et al. (2016) investigated porous polymer film with a similar average pore size to improve the external quantum efficiency of organic light emitting diodes (OLED). Other researcher investigated various shapes and sizes of pores to estimate the overall yield surface (Khdir et al., 2015). The works are focused on porous materials by examining random and orientation pore structures with different volume fractions and shapes.

Porous materials are of significant interest in thermal management materials. Porous materials depend on the microstructural morphology that refers to the shape, size and spatial distribution of the microstructural constituents. Determination of the microstructural properties of porous materials is an essential problem in engineering applications. Studying the relation between pore geometry and spatial distribution using numerical analysis has been proposed by Zhuang et al. (2015). The porous material is designed in macroscopic homogeneous and heterogeneous types, which consist of inclusions, grains, interfaces and cavities. In numerical terms, the porous materials were proposed in representative volume element (RVE) sizes to carry out the parameters of axial ratio, the length of long axis, dip angle and dip direction of the long axis respectively. Heat transport through porous media using the numerical homogenization technique and morphological analysis in microscale of porous materials were developed and published by El Moumen et al. (2015). The 3D pore was designed by random with spherical

and ellipsoidal shapes. In the finite element method, thermal analysis was applied on the representative volume element (RVE) for periodic boundary conditions.

In the theory of effective thermal conductivity of mixtures, the analytical bounds are often used to validate and constrain thermal conductivity models. Realizing the importance a more efficient material design can be achieved through the use of thermal conductivity models. Usage of accurate models is important in order to understand the mechanisms that control thermal conductivity in the polymer. This will result in more efficient material design and could, therefore, reduce the cost of experimental work. Therefore, it is necessary to develop numerical methods for predicting the effective thermal properties. The purpose of this paper is to design the porous polymer of polypropylene (PP) for thermal insulator applications. The pore is developed by using algorithm distribution with various irregular shapes and content.

2. METHODOLOGY

In part of the pores construction technique, the formulation is constructed during the 3D model development. The general principle of the porous structure model is carried out in 3 procedural stages. These procedures involve: pores distribution algorithm as well as a numerical and convergence study implemented as necessary to produce a porous structure.

2.1. Pore Size Distribution Algorithm

The porous material criterion is described in relation to simple pore growth through pore pair partner attachment. The pore pair partner attachment grows when an individual pore launch point (P) is added and attached. The porous construction technique that involves the pore launch point (P) occurs when the porous structure performance occurs and is developed in terms of MATLAB^{TM} commercial coding.

In modeling boundary size parts, there are proposals concerning the various model sizes as activities output for the model size convergence study. The modeling size refers to the sample size which is embedded in several of the pores as porous structures. In this case, the modeling size study is adopted from a previous work by Trias et al. (2006). Which model size (δ) is determined by a ratio between width of model and the pore size and given in Equation 1.

$$\delta = W/D \tag{1}$$

where W denotes the model length from the cubical side and D is the diameter of the pore.

In the cubical model, along the x, y and z axes the pore is divided by imaginary points with the pore diameter as a distance. The number of points design is based on the modeling size in that the greater model size will reveal alot about the content of the number of imaginer points. These imaginer points are positioned at a center of one pore with non-overlapping design. The total number of coordinates is equal to the total number of pores generated. For a simple approach, the pore shape is considered as a shape of a sphere, the length of the modeling size, W, is given in Equation 2.

$$W = (D + d)n \tag{2}$$

Notation D, d and n denote the diameter of pore, the inter-pore distance and the number of points along the axis, respectively. The condition of (D+d) gives the meaning that the inter-pore point distance and inter-pore point always avoids pore-to-pore contact.

The last part of boundary model size analysis is to determine the procedure of pore pair partner. The first step is determining the launch point as pore coordinate in randomly launch. The

launch point (*P*) is developed based on the coordinate points of *x*, *y* and *z*. The random technique design is constructed based on the commercial code of MATLAB™ and the equation for random generation is as follows in Equation 3.

$$t_{i+1} = Ku_i (mod\ n), \qquad i = 1,2,3,\ldots \tag{3}$$

where *K* and *n* are usually integers and mod *n* is the operation that gives, in this case, coordinate points, while t_i is the initial value of iteration time.

Each point comes through moving and finding the nearest attachment point, whose condition is named the 'moving motion point'. The algorithm of the moving motion point is started from the launch point of the particle at coordinate point (P_1), then the distance between the seed point is measured and known as Δd_1. The distance function is used in determining the pair partner which has a closer proximity. Furthermore, the porous pore will be structured through the pair partner formation process. This motion is conducted using the Cartesian coordinates of a spherical (r,θ,α) system, while considering motion attraction. The resultant (r), angle θ, and α are defined as constant when a particle is moving towards the pair partner. The *r* is resultant of the two observed particles, while the angle θ and α denote the angle between two observed particles. The 3D spherical Cartesian coordinates are determined by Equation 4.

$$\begin{aligned} \Delta x &= cos\theta r\ cos\alpha \\ \Delta y &= sin\theta\ r \\ \Delta z &= cos\theta r sin\alpha \end{aligned} \tag{4}$$

2.2. Numerical

The finite element procedures, such as creating geometry, governing equation and meshing are presented to determine thermal conductivity as outlined below.

2.2.1. Generate geometry

The geometric construction is designed with a cubical block that is embedded in a pore structure. A number of several pores are embedded in the cubical block which is determined by the pores content formula. The pores content formula undertaken in this study is using a spherical volume approach to calculate the pores volume, as presented by Equation 5 below.

$$Vol.\% = \frac{(4/3)\pi r^2 (n)}{(w \cdot h \cdot l)} \tag{5}$$

The notation *n* denotes the amount of pores content, while *w*, *h* and *l* are width, height and length of modeling size, respectively.

2.2.2. Governing equations

For thermal study in ANSYS Workbench™ software, the local amount of heat transfer through the material ($\boldsymbol{q_i}$) is computationally determined by solving the steady state equation shown below in Equation 6.

$$q_i^{(e)} = -kA\frac{\partial T}{\partial x} = -kA\frac{(T_j - T_i)}{L^{(e)}} \tag{6}$$

where $\boldsymbol{q}$ is the local amount of heat transfer through the material (*W*), which $\boldsymbol{k}$ is the local thermal conductivity (*W*/*m K*), $\boldsymbol{A}$ is area (m^2) and this is obtained from the local different

thermal (ΔT, K) according to Fourier's Law. This is a perpendicular force passing through the given surface area with a distance from i to j.

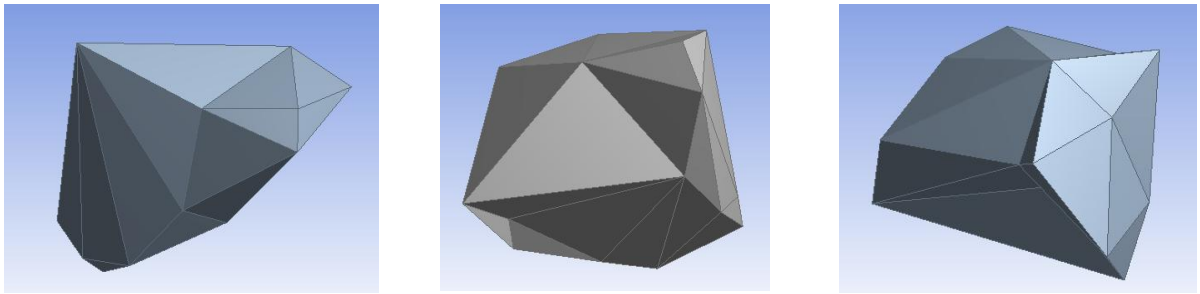
2.2.3. Meshing

The mesh number is above 300,000 to obtain accurate results for thermal conductivity purposes. The grid dependence study of the domain is run for different mesh numbers to check the grid dependency of the model size case. The dependency study is important in the simulation in order to efficiently obtain accurate and cost effective results.

2.3. Pore Shape Development

In this investigation, a random distribution of irregular shaped pores is proposed for thermal analysis. Figure 1 illustrates the various shape probabilities to be considered in the porous numerical model. Three different shapes of pores are studied in the thermal analysis, which are known as Types A, B, and C, respectively. The probability shape is constructed by Voronoi codes formulated in MATLAB™ commercial software as shown in Figure 1. To generate the pore shapes, determine the number of points in a certain space by random dispersion. In this space the sizes will appear as the number of points in a random set. Next, the Voronoi codes formulated in commercial MATLAB™ software will giving the face closed all random point as present the random shape.

To generate the simulated pore shape, first pick points: P1;P2; . . . ;Pi; . . . ;Pn in certain space (pore size) at random locations, according to a Poisson process. Then, construct the three angles of the outer Pi by connecting the points. These three angles will be employing all outer points P1 and perform as an irregular shape. Next, construct the surface on three angles as a closed surface surrounding the irregular shape. As a result of irregular shaped pore, Figure 1 shows the example of random implantation of pore shape. The pore shape is exported to a CAD system for compatibility using a Finite Element Analysis code.



Type A Type B Type C

Figure 1 Probability of three pore shapes

2.4. Volume Fraction Study

The thermal conductivity study is presented by plotting the effect of pores content in the PP material. The pores content is considered in a range of 5%, 10%, 15% and 24% respectively by comparing the volume of PP material. Furthermore, the model size is considered based on the representative volume element (RVE) study.

2.5. Pore Size Study

The thermal conductivity study is presented by plotting the effect of pore size. The pore sizes are varied in a range of 200 nm, 2 μm and 30 μm, respectively. While the volume fraction is fixed at 24 vol.%.

3. RESULTS AND DISCUSSION

3.1. RVE Size Study

Several RVEs are proposed to determine some fixed value of model size. This parameter is used to quantify the thermal conductivity model size for all pore shape types. Figure 2 shows the RVE sizes derived from a thermal analysis study based on various pore shapes. As shown in Figure 2 the thermal conductivity is affected by model size (δ) and pore shape. It indicates that by decreasing the thermal conductivity results in an increase in the RVE size model and it varies according to various pores shapes. The RVE size is selected based on a convergence study from the figures which represent the thermal values in small quantities which fluctuate or to move towards some fixed values. The numerical results found with RVE size model for each case meet with little fluctuation, thus leading to a constant direction when the RVE size is at δ = 5. A similar phenomenon is also indicated in previous works that estimated the RVE size would meet the convergence value (Salahouelhadj & Haddadi, 2010).

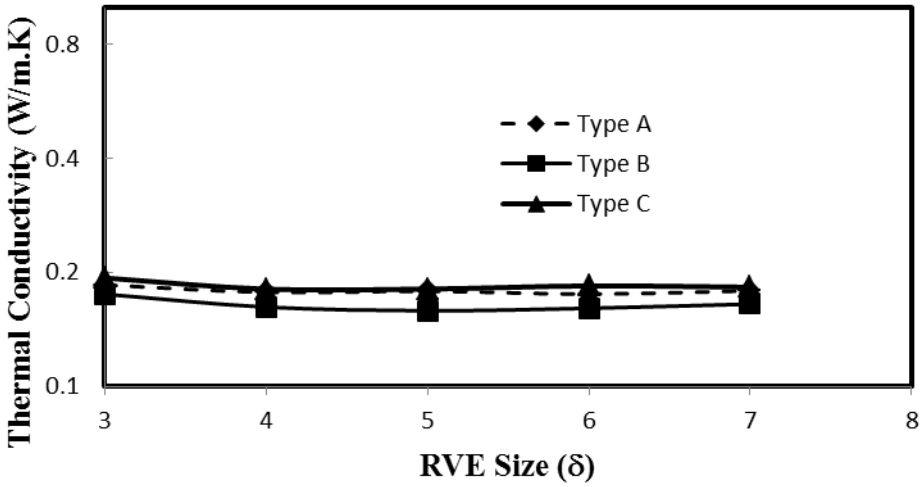
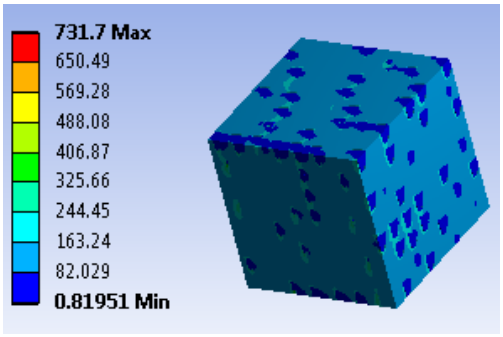
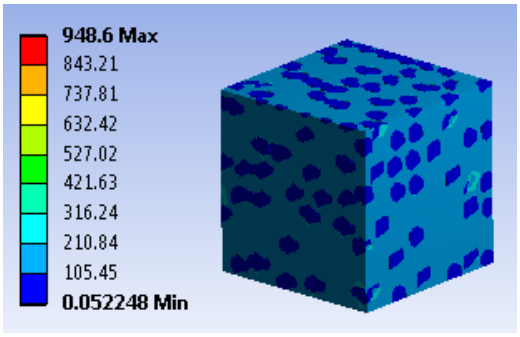


Figure 2 Thermal Conductivity against RVE size model

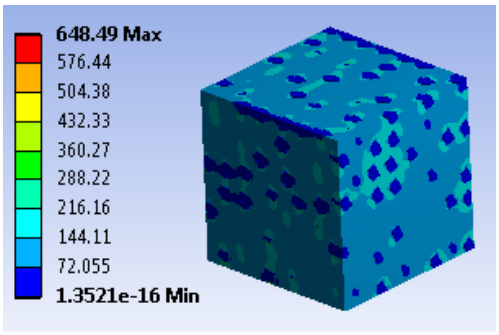
The Poisson technique was implemented to process the random particle dispersions that were positioned at each point as the pore center. The microstructures are considered in non-overlapping pores which have a defined spatial distance between pores. Figure 3 shows an example of the local thermal density distribution in 3D microstructures for different shape types that are discusssed in this investigation. The effect of the pores porosity is investigated in terms of thermal analysis. It was observed that the local heat flux mainly depends on many morphological factors, such as the porosity and the shape of pores. It is noted that in the case of non-overlapping irregular pores shape, the numerical computations are limited to 24 vol.% of the pores content. Distinctive heat flux levels can be found from the legend denoting the figures characterized by extreme different values between the pores and polymer conditions. The heat flux distribution analysis is observed around the pores network as is found by the distinctive contours around the pores. The comparison values can be noted on the legend in that the higher heat flux is found at the polymer body. This indicates a specific direction across the model by following the polymer body. This phenomenon is shown in all models; the overall value of the heat flux indicates a drastic difference when compared to polymer and pores conditions. The heat flux values in the overall models also show different values, due to how the single pore is affected in the overall model. It might be that every single pore has a different density volume that is affected by the heat flux generally.



Type A



Type B



Type C

Figure 3 Local distribution of heat flux for f = 0.24 of non-overlapping cases

3.2. Volume Fraction Effects

The effect of pores content in the PP material is analyzed based on the effective thermal conductivity as shown in Figure 4. The figure presents the various thermal analyses based on various pores content which is a comparison of a numerical model with the analytical models, such as Parallel, Maxwell-Eucken, Hashin-Shtrikman bounds model (Buryachenko, 2006). It appears that the estimated thermal conductivity decreases by increasing the pores content. Type B shows better estimating data than the others due to higher thermal resistance as shown in Figure 4. The numerical results indicate good estimating procedures with resultant analytical values when compared to the Maxwell-Eucken model for lower thermal conductivity. This phenomenon confirms again that the theory of pores density is significantly affected by thermal conductivity. For these reasons, the thermal behavior mainly depends on the distribution type and shape of pores. The estimated thermal conductivity decreases by increasing the pore volume fractions. It should be noted that, the similarity between numerical and analytical data, due to analytical estimates in similar pore sizes when compared with the numerical analysis. However, a disadvantage of the analytical model is found in that it is unable to predict thermal conductivity when the various pores shape effect is applied on the material. The thermal conductivity of pore materials strongly depends on both phases in the matrix and the characteistics of the pores themselves. The thermal conductivity considered for the matrix phase ranges from 0.1 to 0.2 W/m K and for pores 0.024 W/m K respectively. For a higher particles volume fraction and a higher contrast of phases, the comparison can give a useful estimate of the effective properties.

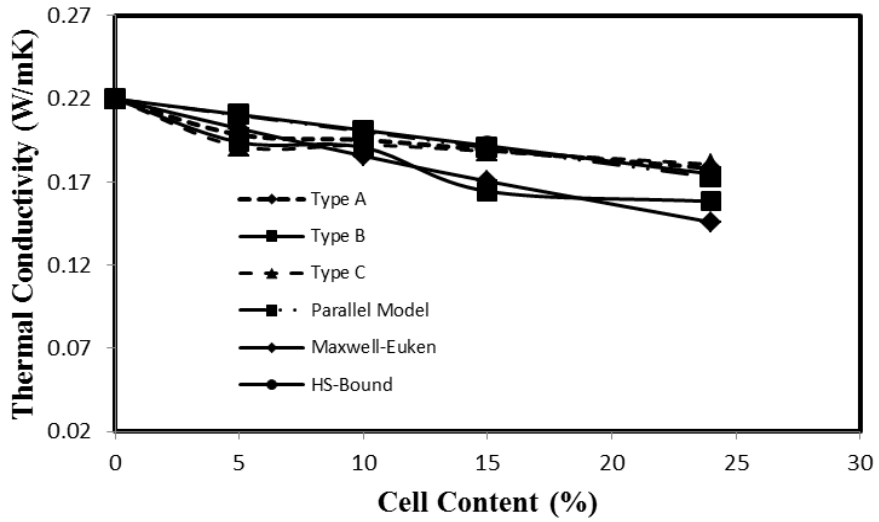


Figure 4 Thermal conductivity against pore content

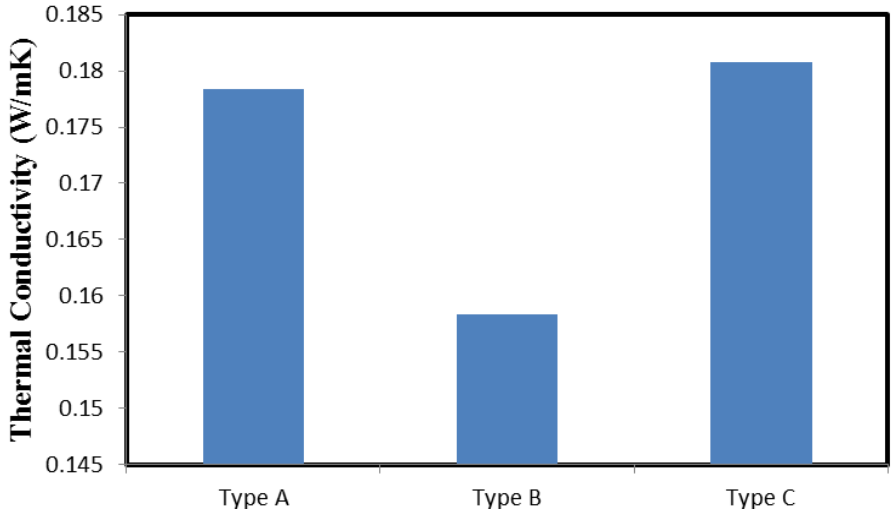


Figure 5 Thermal conductivity against pore type at 24 vol.% of pore content

Figure 5 presents the effect on pores shape compare to thermal conductivity at 24 vol.% of pores content. Type B shows higher thermal resistance with similar microstructure patterns when compared to the others, which indicates that a Type B single pore has a higher volume density compared to the others.

3.3. Pore Size Effect

In order to obtain good predictions of the pores material in the thermal application, the size of the pore is also discussed in this part. The modeling is simulated at 24 vol.% of volume fraction with $\delta = 5$ for model size. The results show that the pore size represents an insignificant effect on the thermal conductivity of the porous material as shown in Table 1. This phenomenon is similar to data reported by previous work in that the mean pore diameter only weakly affects the results (Khan & Straatman, 2016).

Table 1 Thermal conductivity of multiple shape pores against size

Size (μm)	Type A (W/mK)	Type B (W/mK)	Type C (W/mK)
0.2	0.178306	0.15933	0.180784
2	0.178357	0.15838	0.180716
30	0.178225	0.158346	0.180815

4. CONCLUSION

The algorithm of pore distribution models for porous material and RVE size for insulator applications through establishing the effect of pore shape, number and size has been investigated. Moreover, the pore shape has been developed successfully to carry out the investigation on the nature of pore shapes by the Vorronoi method. This algorithm of pore distribution is used potentially to predict thermal conductivity of the PP polymer for insulator application. In this work the findings indicated that the volume of pores results in a significant effect in decreasing the thermal conductivity. It was proven that the thermal conductivity was affected by the additional pore content. In addition, the shape also affected the porous material in terms of thermal conductivity, since every single pore resulted in a different single density volume. Otherwise, the variation in pore diameter weakly affected the results in thermal conductivity. The information obtained from these results will provide a useful platform for further study in experimental works.

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