EFFECT OF MORPHOLOGICAL PARAMETERS AND PHYSICAL MATERIAL PROPERTIES ON EFFECTIVE THERMAL CONDUCTIVITY OF HETEROGENEOUS RANDOM TWO-PHASE MATERIAL

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Effective Thermal Conductivity ETC of some complex materials is analyzed and compared to analytical results of Maxwell-Eucken (ME) and self-consistent estimation (SC). Finite element technic is used for numerical homogenization calculations with appropriate imposed boundary conditions to the representative volume elements (RVE) of the materials. Complex material and particulate reinforced material with spherical inclusions are considered. Three volumes fraction were studied in this paper. The first objective is to make a comparison between these microstructures to established a relation between their morphological parameters and their thermal conductivity. The second is to demonstrate the efficiency of the analytical model to predict with good precision the thermal conductivity ETC properties of material.

Keywords: heterogeneous material, thermal conductivity, numerical homogenization.

1. Introduction

Current expansion of the use of new materials in chemical, mechanical, geological applications prompted the development of the study of their properties, for this reasons many studies on the determination and predication of thermoelastic properties have been improved and progressed in the case of heterogeneous materials [1-3].

During the first years, analytical estimates of thermal properties have been improved and published in the case of composite materials. Progelhof et al. [4] present an analysis of approaches of prediction the thermal conductivity of heterogeneous material. Numerical homogenization technique, based on the concept of representative volume elements (RVE), is widely used to estimate and analyze composite materials to obtain thermal properties. In many research's papers, finite element method is used to comprehend the consequence of amount of

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reinforced particles on the thermal performance of composites material. Qiang et al. in [5] studied the numerical calculus of thermal conductivity ETC with (FEM). The effects of the distribution, orientation and shape of the pores on thermal conductivity have been investigated by Bakket et al. [6]. Bolot et al. in [7] study the heat transfer through a porous medium by computational methodology. El Moumen et al. in [8] studied the relationship between the morphological parameters of microstructures and their effective thermal conductivities. Fedaoui et al. [9] and Boutaani et al. [10] investigate the effect of morphological parameters in the effective thermal and mechanical propreties of different composite material by finite element method. In the paper of Chaibainou et al. [11], Al-SiC composite material was subject of the numerical computation by finite element method and a comparison with experimental results was done.

Chih-Chun Chang et al. in [12] determine the effective thermal conductivity of composite materials by combining a packing algorithm of generating materials with finite difference solver. Chuan-Yang Zhu et al. in [13] studied the thermal conductivity of certain reinforced materials and they compare some analytical models proposed in literature. After they propose an extension of the Meredith and Tobias model. This model is able for predicting the thermal conductivity of cloudy multiphase composites by various spherical particles with variable volume fractions.

In [14] HUI studied the thermal insulation performance of using insulating cementitious foam plates with increasing amount contents of hollow glass microspheres (HGM) by the transient plane source method. The results obtained show that the ETC value of the foam decreases with the increase of the size of (HGM),

It can see that numerical predictions show that the coefficient of thermal conductivity of the foam increases with increasing thermal conductivity.

In the present work, the influence of phase form on thermal conductivity is investigated using the FEM method. By the application of specific boundary conditions, a homogenization technique, coupled with FEM finite element simulations was used. Comsol multiphysics software [10] was used in all the computations. Two different materials are considered, one with complex shapes for the second phase and the second with embedded spherical particles in a matrix. The equivalent morphology concept is presented and proposed here to substitute the biphasic material of complex shape by a simple two-phase composite composed of spherical inclusions embedded in the matrix. Numerical results were compared to analytical solutions, such as the Maxwell-Eucken (ME) models of [15] and the self-consistent estimate (SC) of [16].

2. Numerical homogenization approach

For this work, all the basic concepts of the homogenization in composite material of the prediction of effective thermal properties addressing in our case the

ETC effective thermal conductivity, using the method presented by [17] and founded on the Finite element method FEM, are approved.

3. Automatic design and generating of material

The methodology used in Fedaoui et al. in [9], Boutaani et al. [10] and Laid et al.[11] is adopted in this work for the design and generating of numerical material. The estimation of the ETC of two-phase composite materials by numerical simulation is presented in this work. By the use of the RSA particle random position generation algorithm. For Numerical Computations, Comsol Multiphysics software was the tool for the computation of the thermal effective conductivity properties ETC, see figure 1.

For simplify the prediction of this properties for a large and big volume of material, computations were accomplished by the choice of a minimal Representative Volume Element (RVE) for the two cases of study. The first composite randomly filled with spherical particles and the second material with complex morphology.

The RSA algorithm define the locations of the spherical particles for a given particles amount, in a cubic material form taken like matrix. A distance between particles must be imposed to guarantees that there is no intersect with the others particles already created. The generation process will not stop until the inclusion numbers or the volume fraction of the particles are reached. Second complexes material is generated by using the Musgrave Texture of Blender software.

Fig. 2 gives a representation of different materials inclosing a random distribution and orientation of spherical particles or the complex material with overlapping phases for different volume fractions. A contrast of 12.5 was chosen between the different material phases for the two materials see Table 1 and 2. $\emptyset_i$ and λ_i represents respectively the proportion and the thermal conductivity of the second material (spherical particles or the complex material phase). $\emptyset_m$ and λ_m is the proportion and thermal conductivity of the polymer matrix.

Table1

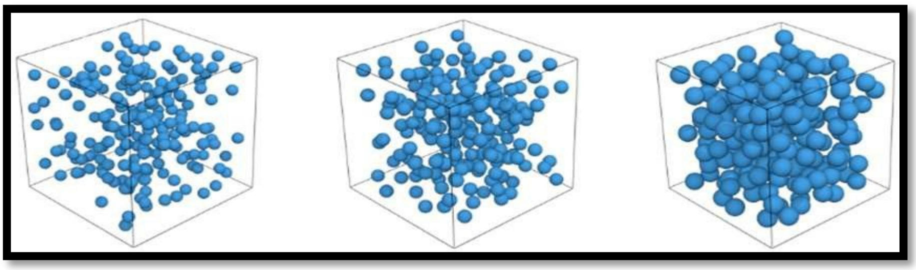
Composites materials properties

Material	Case	Volume fraction for matrix and inclusions
Complex Two-Phase material	**1**	φ =95%, ϕ_1 = 5%
	2	φ =90%, ϕ_1 =10%
	3	φ =80%, ϕ_1 =20%

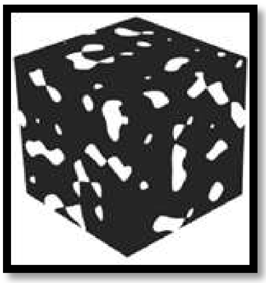
Table2

Thermal conductivity properties

	$\lambda_m(W/mK)$	$\lambda_i(W/mK)$	Contrast
Case 1	0.3	0.024	12.5



a)



b)

Fig. 1. Generating Process of microstructures of different volume fractions, a) spherical morphology and b) the complex morphology.

4. Mesh generation and boundary conditions

COMSOL Multiphysics software can mesh automatically your model (simple one or complexes) and streamline the process of meshing your model or it is possible to choose to build a specific mesh manually.

For a good convergence, an acceptable mesh density is adopted in all the computations. With Comsol great abilities, it is possible to do this through a physics-controlled or user-controlled mesh sequence type. There are many meshing options, settings, tools, and generators to create an optimal mesh for any model geometry and analysis.

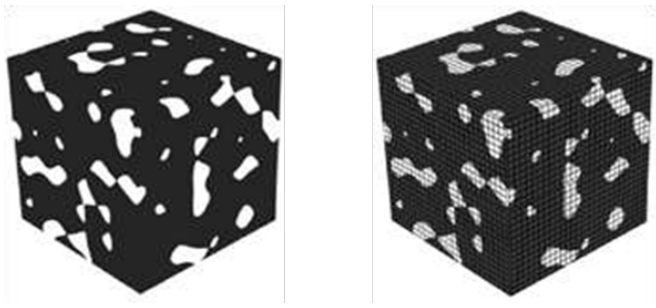


Fig 2 : Example of a material with a complex two-phase structure: a) 30% complex structure, b) 3D mesh [10]

Specific boundary conditions are imposed by the use of different temperature between the two opposite faces of the volume element RVE taken, see fig.3.

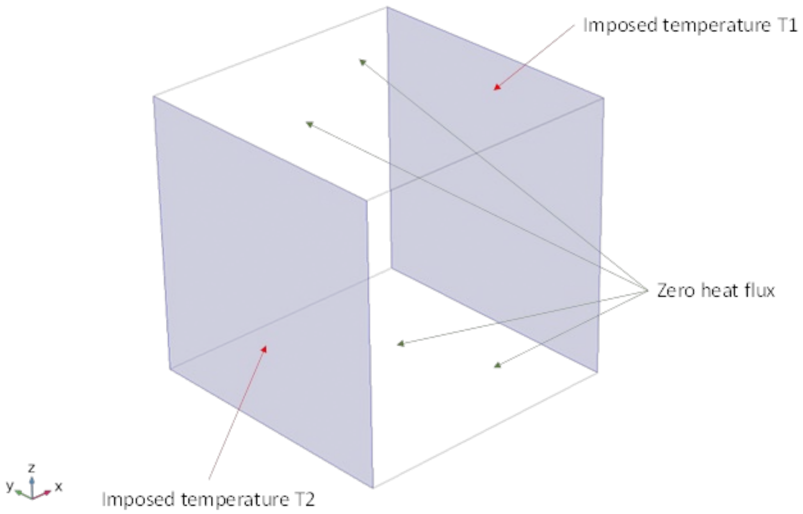


Fig 3: volume element RVE and boundary conditions through its surfaces

5. Conduction Fourier's law

Local heat flux density q is given by expression that result from the product of thermal conductivity λ and the negative local temperature gradient $-\nabla T$.

$$q = -\lambda \nabla T \tag{1}$$

In the case of a composite material, the heat flow that passes through this material (matrix and particles) depends essentially on the thermal conductivities values of these components, on the volume content and the elements distribution. Effective thermal conductivity ETC of composite is considered like the principal thermal properties, which define the thermal comportment of composites material under thermal loading.

6. Theoretical models of prediction

Theoretical models of prediction were developed before the great development in numerical tools with finite elements technics, for the approximation or prediction of effective elastic and thermal properties for multiphase materials. The ETC is the most essential properties in new material design.

7. Model of Self-Consistent

The self-consistent model for the prediction of ETC is the positive solution of the equation proposed by Bruggeman (1935). This model is also known under the name of EMT (Effective Medium Theory, Landauer (1952).

$$\frac{\lambda_1-\lambda^{eff}}{\lambda_1+2\lambda^{eff}}(1-p)+\frac{\lambda_2-\lambda^{eff}}{\lambda_2+2\lambda^{eff}}p=0 \quad (2)$$

The solution is presented as follows:

$$\lambda^{eff}=\frac{1}{4}\left[(3p-1)\lambda_1+\lambda_2(3(1-p)-1)+\sqrt{[(3p-1)\lambda_1+\lambda_2(3(1-p)-1)]^2+8\lambda_1\lambda_2}\right] \quad (3)$$

where λ_i with i indicate the thermal conductivity of every constituent and p the volume fraction.

8. Maxwell's models

Maxwell's models are widely used in predicting and estimating the effective properties of composite materials. This is due to their great adaptation to develop such models of mixtures in general. In particular, it is noticed that this model is usually used, because it does not require any geometric parameter or spatial distribution information of the constituents of the composite or of the mixture. In this approach, it is assumed that the composite in question consists of spheres randomly dispersed in a continuous medium [9]. Effective thermal conductivity λ^{eff} is then given by:

$$\lambda^{eff}=\lambda_2\frac{2\lambda_2+\lambda_1-2(\lambda_2-\lambda_1)p}{2\lambda_2+\lambda_1+(\lambda_2-\lambda_1)p} \quad (4)$$

where λ_i with i the thermal conductivity of every component and p the corresponding amount.

9. Results and discussion

In this part, different realizations of the two composites material are produced to be used in computations of their physical properties ETC. For the computation of thermal effective properties of random materials, numerical technique coupled with RVE established by kanit et al in [17] is adopted. The representative volume elementary (RVE) is defined as the minimal material size that permits the determination of the effectives properties with only one realization.

First, study of effective thermal conductivity λapp for the two composites considered in this work is presented and compared. Three-volume fraction are taken like examples for the study.

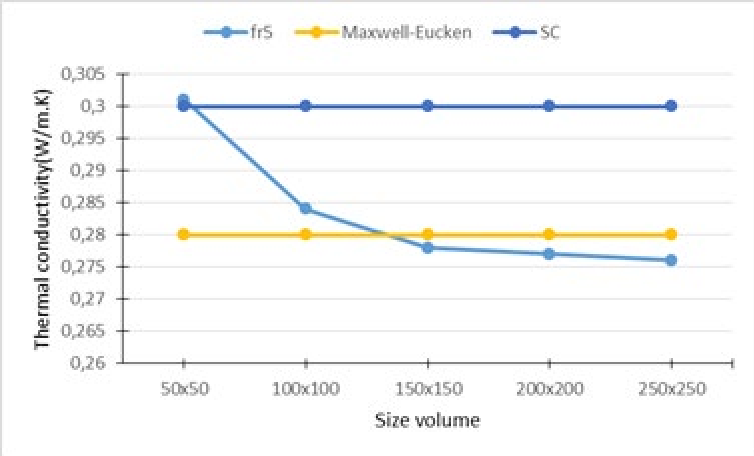


Fig 4. Thermal conductivity fluctuation λapp for complex structure with change of volume size (case 1)

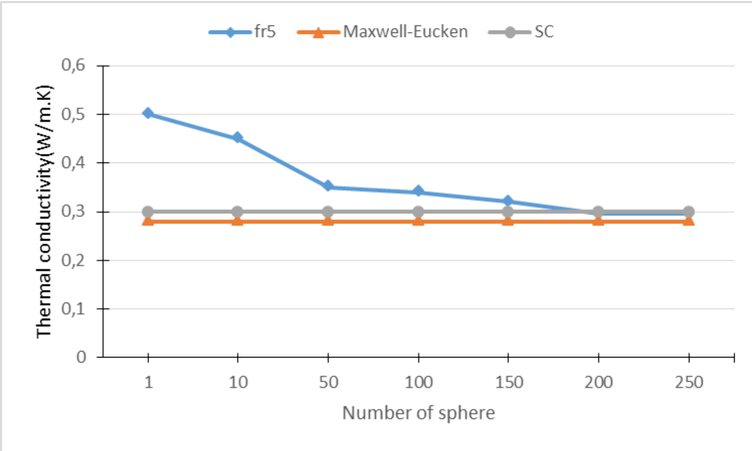


Fig 5. Thermal conductivity fluctuation λapp for spherical structure with a change in number of sphere (case 1)

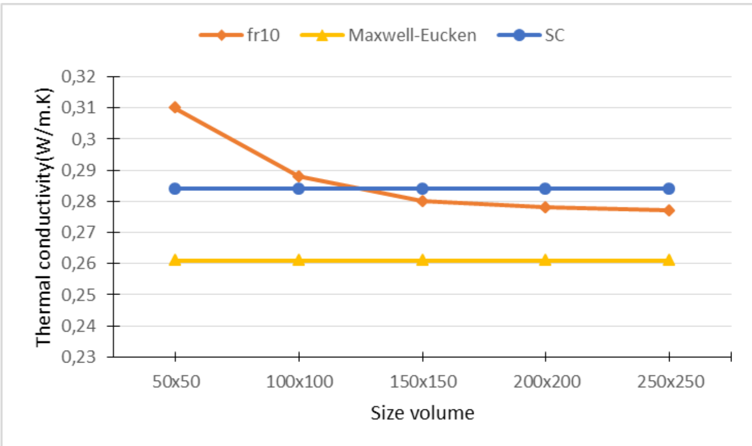


Fig 6. Thermal conductivity fluctuation λ^{app} for complex structure with change of volume size (case 2)

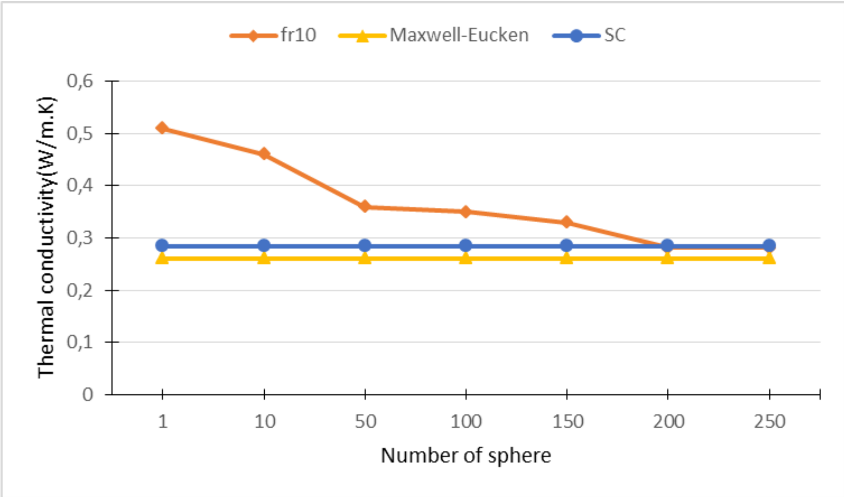


Fig 7. Thermal conductivity fluctuation λapp for spherical structure with a change in number of sphere (case 2)

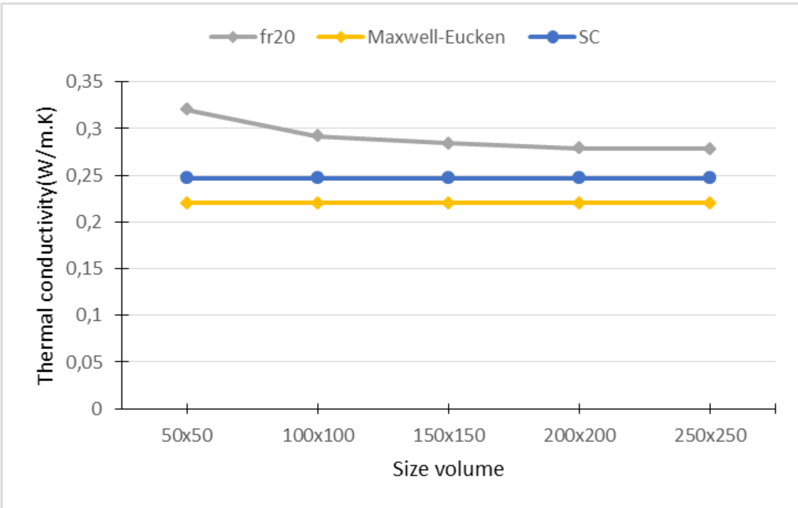


Fig 8. Thermal conductivity fluctuation λapp for complex structure with change of volume size (case 3)

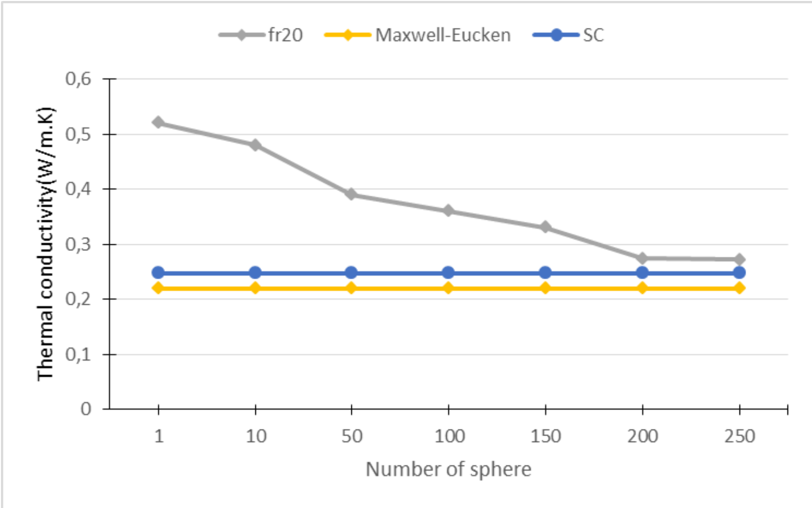


Fig 9. Thermal conductivity fluctuation λapp for spherical structure with a change in number of sphere (case 3)

10. Fitness of analytical approach to predict the thermal properties

From this study, the capability of some analytical method of estimation of thermal properties of some material realization is improved. From figures 1 to 9, one can note that the computations results of thermal conductivity are agree well with the results estimated with the self-consistent model.

The self-consistent model provides a good result for the two cases of spherical and complex material. The effect of volume fraction in all the materials considered here is insignificant.

11. Effect of material morphology on the heat transfers

The morphology and the disposition of the constituents of composites plays a large role in the effective properties of the material. From figures 3-7, results obtained by simulation for the cases studied here improve these theories. For the same volume fraction, the effective thermal conductivity depends on the morphology and the spatial distribution of the constituents making up the material.

An important remark concerning the results obtained for the cases of small volumes, the value are dissimilar from the effective properties found in the cases of large sizes, El Moumen et al in [18] for elastic properties and Kaddouri et al in [19] for the physical properties.

12. Effective thermal conductivity dependence on particle volume fraction

For many years, numerous scientist have explored filler volume fraction and morphology effects on effective thermal conductivity ETC of composite [20, 21]. With the intention of search the effect of this point on the ETC values, three volumes fractions of spherical inclusions and second phase for the complex material were investigated.

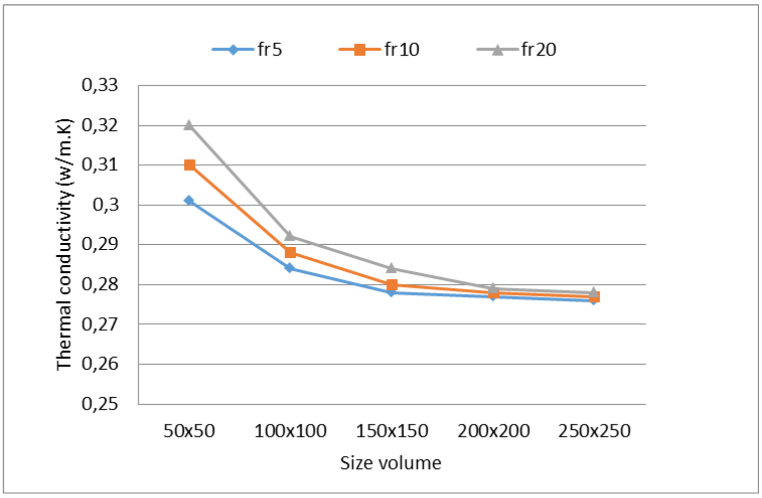


Fig 9. Thermal conductivity variation of λapp for a complex structure with change of volume size

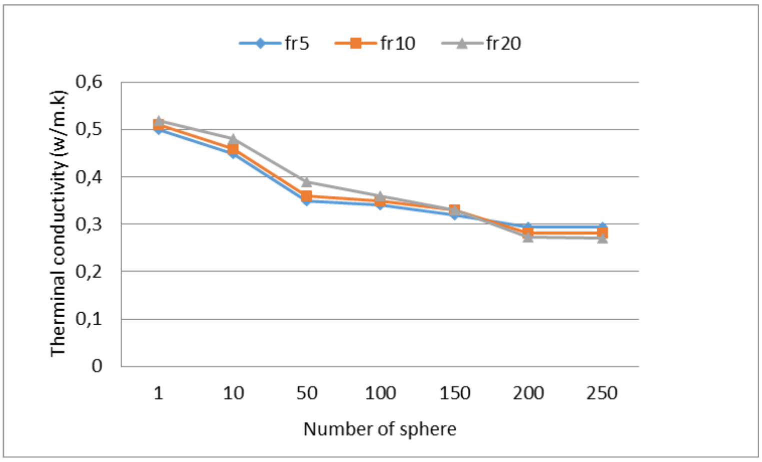


Fig 10. Variation in the thermal conductivity λapp for a spherical structure with a change in number of sphere

The morphology and the disposition of the constituents of composites plays a large part in the effective properties of the material. It is observed that from figures 9-10, the results obtained by simulation for the two cases studied here improve these theories. For the same reinforced portion, the effective thermal conductivity depends on the morphology and the spatial distribution of the constituents making up the material.

It can be noted that from figures 9 and 10, that the ETC fluctuation of the two composite cases increase with the increase of volume fraction of spherical inclusion in the first composite or the second phase for the complex material.

13. Conclusions

The design of new efficient, smart and recyclable materials for new applications like Aerospatiale, Medical and Industrial requires knowledge of theirs properties in the early phase of design. Composite materials are widely used today for theirs great properties. The main properties of the materials is effective thermal conductivity. Effective thermal conductivity of the composites material is affected by some factors, for that in many cases it is complicated to estimate ETC exactly.

In this paper, numerical computation of effective thermal conductivity is used to predict and compare this property for two cases of composite material. One reinforced with randomly distributed spherical inclusions and the second is a complex two phase material. RSA algorithm was used for generating 3D material with arbitrary spherical particle distributions in the matrix.

It can be noted that the ETC fluctuation of the two composite cases increase with the increase of volume fraction of spherical inclusion in the first composite or the second phase for the complex material.

The morphology and the disposition of the constituents of composites plays a large role in the effective properties of the material. Results obtained by simulation for the cases studied here improve these theories. For the same volume fraction, the effective thermal conductivity depends on the morphology and the spatial distribution of the constituents making up the material.

From this study, the capability of some analytical method of estimation of thermal properties of some material realization is improved. One can note that the computations results of thermal conductivity are agree well with the results estimated with the self-consistent model. The self-consistent model provides a good result for the two cases of spherical and complex material. The effect of volume fraction in all the materials considered here is insignificant.

For the perspectives, it is envisaged the experimental tests for the comparison with these results by the use of a real material and particles.

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