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Thermal Conductivity Coefficient Of Particulate Composites As Defined By The Particle Arrangement

J. Venetis

School of Applied Mathematics and Physical Sciences, NTUA
Email: johnvenetis4@gmail.com

E. Sideridis

School of Applied Mathematics and Physical Sciences, NTUA, Section of Mechanics
5 Heroes of Polytechnion Avenue, GR – 157 73 Athens, Greece
Telephone: +30 210 – 7721224 Fax: +30 210 – 7721302
Email: siderem@mail.ntua.gr

Abstract
A theoretical method to estimate the thermal conductivity coefficient of particulate composites is presented in this work. The mathematical formulation is performed by considering the equation of unsteady state heat conduction. Hence, the obtaining of a closed – form solution to this equation can lead to the theoretical evaluation of thermal conductivity coefficient provided that the heat capacity and the density of the overall material, which is macroscopically considered as homogeneous, are known beforehand. In addition, we assume that the particles inside the matrix are insulated and therefore the thermal conductivity of each particle is zero. Thus, the geometrical models for the particle distribution which are adopted here contain at least one impenetrable layer.

Keywords Thermal conductivity coefficient, particulate composites, particle distribution, heat conduction

Introduction

A particularly important property of composite materials is the degree of thermal conductivity, which is measured by the thermal conductivity coefficient. This property plays a critical role in the design of electronic packaging used for micro electronic devices. Composites used for the structural components of aircraft or other technological systems that are subjected to extreme environmental conditions, need a low thermal conductivity coefficient in order to be sound under a change of temperature. The objective of the majority of microstructural models is actually the reproduction of a Representative Volume Element (RVE) of the composite at a microscopic scale, so that a solution be achieved and compared with experimental results. Such a fundamental problem is the determination of thermal conductivity coefficients within the composite at various filler volume fractions when mutual interaction of perturbation fields of adjacent inclusions occurs. The microstructural models are usually based on the assumptions that a regular geometric form is applicable for the inclusions usually a sphere or cylinder [1]. Various theoretical approaches have been proposed to yield the thermal conductivity for filler–matrix systems. The Maxwell theoretical model is the basis of many of these models. This fundamental model uses potential theory to obtain an exact solution for the conductivity of a system with spherical, non – interacting particles in a continuous matrix [2]. Besides, the Rayleigh–Maxwell model is effective for a two-phase dispersion of spherical particles in continuous medium for entire range of filler concentration in composites [3]. However, the above mentioned models though their prominent mathematical analysis, mainly concern non – interacting spherical particles. In this context, a lot of research work has been carried out for the determination of thermal constants of particulate composites and for the investigation of the effect of various parameters such as filler – matrix interaction. Specifically, in Ref. [4], the thermal expansion response of particle – filled polymer matrix composites is studied by the use of a micromechanical model, consisting of epoxy matrix filled with solid – sphere or hollow – sphere silica particles. In this considerable work, various finite element analyses based on the axisymmetric unit-cell model, with two types of filler arrangement are also performed. However, the effects of particle spatial distribution on the average composite thermal expansion coefficient are small. Meanwhile, Hashin [5], Herve [6] and Qiu and Weng [7] used an interesting replacement technique to find the thermal expansion coefficient of a particle inclusion surrounded by an inhomogeneous interphase layer. The same technique was also used by Lombardo [8] to find the thermal expansion coefficient of a particulate composite with inhomogeneous interphase. The idea was originated by Garboczi and Berryman [9] who also mapped a particle and surrounding interphase onto an effective homogeneous particle although in their work the interphase was assumed to be homogeneous. On the other hand, Felske [10] investigated the effective thermal conductivity of composite sphere in a continuum medium with conduct resistance, whereas Karayacoubian et al [11] used two simple theorems to establish thermal resistance – based bounds for the effective conductivity of composites. Khan and Muliana [12] introduced a micromechanical model for predicting thermal expansion coefficient and thermal conductivity of composites having solid spherical particle reinforcements, while Sideridis et al [13, 14] proposed closed – form solutions towards the estimation of elastic modulus and thermal expansion coefficient of this type of composites by considering the influence of particle arrangement. Nevertheless, these models are not consistent with the conclusion drawn by Yin and Sun [15] where it is mentioned that the particle interactions make no contribution to the effective bulk modulus, a result which is in agreement with some other models. In this investigation, we shall perform a qualitative estimation of the thermal conductivity coefficient from a Mathematical Physics standpoint taking into account the arrangement of the particles and hence a possible effect of their interaction. To this end, two reliable microstructural models of a regular geometry which are simulated in a 3 - phase and a 4 - phase spherical RVE respectively, will be adopted. Evidently, these theoretical models which formulate the particle distribution contain one or two impenetrable layers.

Remarks on two basic theoretical models for the microstructure of particulate composites

It is well known that the majority of microstructural models aim at the reproduction of the basic cell or representative volume elements (RVE) of the composite at a macroscopic scale in order to obtain a solution. Such a fundamental open problem is the determination of mechanical stresses developing within the composite at high volume fraction of inclusions when interaction between perturbational fields of adjacent inclusions occurs. These models are usually based on the following assumptions:

i) A regular geometric form is adopted for the inclusions usually a sphere or cylinder. Here, the particles are perfectly spherical in shape.

ii) Regular geometry and topology are adopted for the model. Experimental models can be plane or spatial. It is obvious that a three dimensional structure is synonymous with a composite material structure.

iii) The inclusions and the matrix are elastic, isotropic and homogenous and their distribution is uniform so that the composite may be regarded a quasi – homogeneous isotropic material.

iv) The deformations applied to the composite are small enough to maintain linearity of stress – strain relations.

The model adopted in Fig.1 represents a three – dimensional system capable of simulating real particle composites. Assuming equal inclusions, which is not necessarily the case in reality, the volume fraction, U_f, of the fillers in the continuous matrix is given in terms of the ratio $2\,r_f\,/\,l$ where r_f is the filler radius and l the inter – centre distance. The maximum value of this ratio and the maximum value of the volume fraction depend on the relative position of the spherical inclusion.

The inclusions occupy the eight vertices of a cube or that they are placed at the middle of each one of the twelve sides of the cube. In order to make a more refined analysis a cubic model with no spherical inclusion in its centre is adopted as basis.

Then, three models can be considered as derived from the following distributions:

1) A cubic with 8 inclusions at the eight vertices of the cube.

2) A cubic with 12 inclusions at the mid-space of the sides of the cube.

3) A cubic with 6 inclusions at the centers of the faces of the cube.

Apparently, these models can create three combinations.

A cube of side 2 l surrounds the cube of side l and thus constitutes the unit cell with it. This array continues in all material. Thus, the variations of the model designated as M_1, M_2, M_3 respectively are obtained. The representative volume element, RVE, is illustrated in Fig.1.

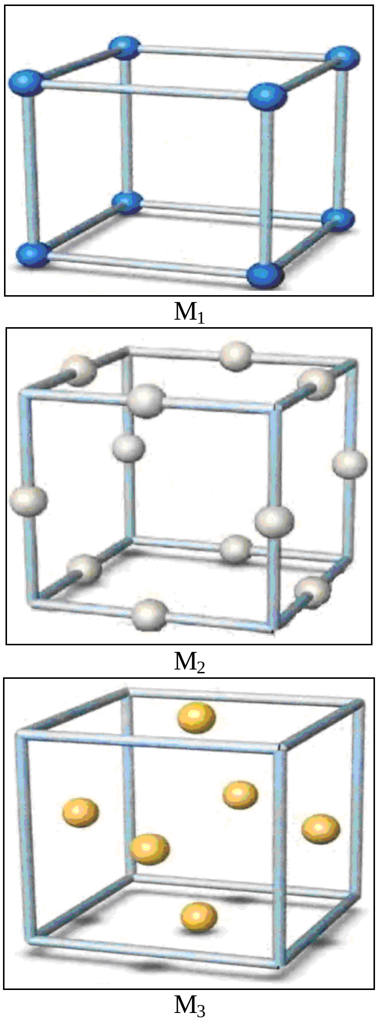

Fig. 1 Typical cubic models a) Simple cubic model, b) Side centered cubic model, c) Face centered cubic model

To facilitate the initiated analysis, the cubic RVE is transformed to a spherical one consisting of three phases, as it can be seen in Fig.2.

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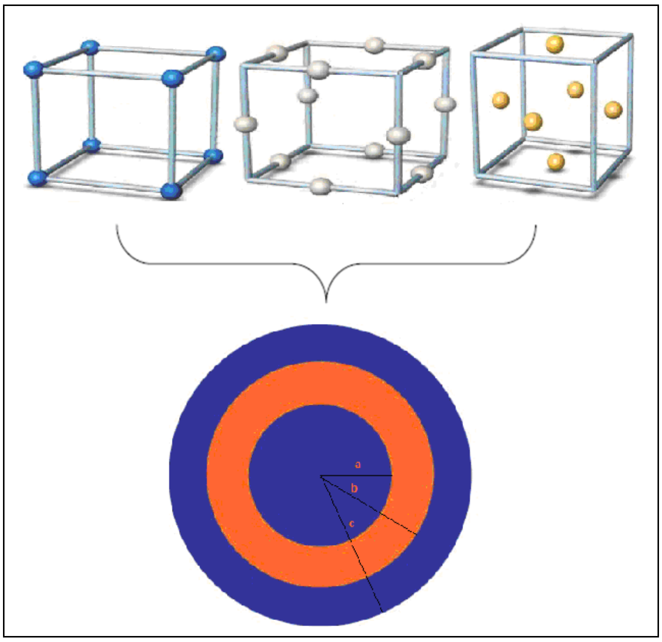


Fig. 2 Transformation of the cubic RVE to an equivalent spherical one

Hence, in regards to the first spherical model where the inclusions are on the vertices of the cube we can write out,

$$V_{2l} = (2l)^3 \quad \Rightarrow \quad V_{2l} = 8l^3 \qquad (1)$$

and

$$U_f = \frac{8\frac{4}{3}\pi r_f^{\,3}}{(2l)^3} \quad \Rightarrow \quad U_f = \frac{32}{24l^3}\pi r_f^{\,3} \quad \Rightarrow \quad l = r_f\sqrt[3]{\frac{4\pi}{3U_f}} \qquad (2)$$

Thus, to the volume of cube with side $2l$, in the first model there corresponds the volume of sphere with radius c, and therefore

$$2l^{\,3} = \frac{4}{3}\pi c^3 \quad \Rightarrow \quad c = l\sqrt[3]{\frac{8\cdot 3}{4\pi}} = l\sqrt[3]{\frac{6}{\pi}} \qquad (3)$$

Hence we deduce that

$$c = r_f\sqrt[3]{\frac{4\pi}{3U_f}}\sqrt[3]{\frac{6}{\pi}} = r_f\sqrt[3]{\frac{8}{U_f}} \qquad (4)$$

Next, referring to the volume of cube with side l the distance between its centroid and an arbitrary vertex is estimated as

$$w = l\frac{\sqrt{3}}{2} \qquad (5)$$

The second phase of the composite consists of the inclusions and therefore

$$\frac{4}{3}\pi(b^3 - a^3) = 8\frac{4}{3}\pi r_f^{\,3} \quad \Rightarrow \quad (b^3 - a^3) = 8r_f^{\,3} \qquad (6)$$

Hence, we can deduce that

$$\frac{4}{3}\pi(b^3 - w^3) = \frac{4}{3}(w^3 - a^3) \quad \Rightarrow \quad (b^3 + a^3) = 2w^3 \qquad (7)$$

Adding by members eqns. (6) και (7), one finds

$$b = \sqrt[3]{w^3 + 4r_f^{\,3}} \qquad (8)$$

while subtracting them by members it follows

$$\alpha = \sqrt[3]{w^3 - 4r_f^{\,3}} \qquad (9)$$

Meanwhile, in the second model, we have considered that there exist totally 12 inclusions in the middles of all sides of the cube. Hence, the filler content U_f is evaluated as

$$U_f = \frac{12\frac{4}{3}\pi r_f^{\,3}}{(2l)^3} \quad \Rightarrow \quad U_f = \frac{48}{24l^3}\pi r_f^{\,3} \quad \Rightarrow \quad l = r_f\sqrt[3]{\frac{2\pi}{U_f}} \qquad (10)$$

In continuing, we take into account that to the volume of cube with side $2l$ in the second model there corresponds the volume of a sphere with radius c, and therefore

$$2l^{\,3} = \frac{4}{3}\pi c^3 \quad \Rightarrow \quad c = l\sqrt[3]{\frac{8\cdot 3}{4\pi}} = l\sqrt[3]{\frac{6}{\pi}} \qquad (11)$$

Hence it follows,

$$c = r_f\sqrt[3]{\frac{2\pi}{U_f}}\sqrt[3]{\frac{6}{\pi}} = r_f\sqrt[3]{\frac{12}{U_f}} \qquad (12)$$

Let us consider again the volume of cube with side l. Then the distance between its centroid and an arbitrary vertex is estimated as

$$w = l\frac{\sqrt{2}}{2} \qquad (13)$$

The second phase of the composite consists of the inclusions and therefore

$$\frac{4}{3}\pi(b^3 - a^3) = 12\frac{4}{3}\pi r_f^{\,3} \quad \Rightarrow \quad (b^3 - a^3) = 12r_f^{\,3} \qquad (14)$$

Hence, we can deduce that

$$\frac{4}{3}\pi(b^3 - w^3) = \frac{4}{3}(w^3 - a^3) \quad \Rightarrow \quad (b^3 + a^3) = 2w^3 \qquad (15)$$

Thus, adding and subtracting by members eqs. (14) and (15) respectively, one obtains

$$b = \sqrt[3]{w^3 + 6r_f^{\,3}} \qquad (16)$$

$$\alpha = \sqrt[3]{w^3 - 6r_f^{\,3}} \qquad (17)$$

Next, the third model contains totally 6 inclusions in the middles of all faces of the cube. Hence, the filler content U_f is calculated as

$$U_f = \frac{6\frac{4}{3}\pi r_f^{\,3}}{(2l)^3} \quad \Rightarrow \quad U_f = \frac{24}{24l^3}\pi r_f^{\,3} \quad \Rightarrow \quad l = r_f\sqrt[3]{\frac{\pi}{U_f}} \qquad (18)$$

Then, we take into account that to the volume of cube with side $2l$ there corresponds the volume of a sphere with radius c, and therefore

$$2l^{\,3} = \frac{4}{3}\pi c^3 \quad \Rightarrow \quad c = l\sqrt[3]{\frac{8\cdot 3}{4\pi}} = l\sqrt[3]{\frac{6}{\pi}} \qquad (19)$$

Hence it implies,

$$c = r_f \sqrt[3]{\frac{\pi}{U_f}} \sqrt[3]{\frac{6}{\pi}} = r_f \sqrt[3]{\frac{6}{U_f}} \quad (20)$$

Also, similarly to the presentations of the previous models the distance w is now estimated as

$$w = \frac{l}{2} \quad (21)$$

The second phase of the composite consists of the inclusions and therefore

$$\frac{4}{3}\pi(b^3 - a^3) = 6\frac{4}{3}\pi r_f^{\ 3} \quad \Rightarrow \quad (b^3 - a^3) = 6r_f^{\ 3} \quad (22)$$

Hence it follows

$$\frac{4}{3}\pi(b^3 - w^3) = \frac{4}{3}(w^3 - a^3) \quad \Rightarrow \quad (b^3 + a^3) = 2w^3 \quad (23)$$

Thus, adding and subtracting by members ens. (22) and (23) respectively, one obtains

$$b = \sqrt[3]{w^3 + 3r_f^{\ 3}} \quad (24a)$$

$$\alpha = \sqrt[3]{w^3 - 3r_f^{\ 3}} \quad (24b)$$

In the sequel, one should state the following restrictions arising from the geometry of the above mathematical formulation.

First model:

$$a > 0 \Rightarrow \sqrt[3]{w^3 - 4r_f^3} > 0 \Rightarrow w^3 - 4r_f^3 > 0 \Rightarrow$$

$$\left(l\frac{\sqrt{3}}{2}\right)^3 - 4r_f^3 > 0 \Rightarrow \left(r_f \cdot \sqrt[3]{\frac{4\pi}{3U_f}} \cdot \frac{\sqrt{3}}{2}\right)^3 - 4r_f^3 > 0$$

$$\Leftrightarrow \frac{4\pi}{3U_f}\left(\frac{\sqrt{3}}{2}\right)^3 > 4 \Rightarrow \frac{\pi}{3U_f}\left(\frac{\sqrt{3}}{2}\right)^3 > 1 \Rightarrow$$

$$U_f < \frac{\pi\sqrt{3}}{8} \Rightarrow U_f < 0.68017 \quad (25a)$$

$$b < c \Rightarrow \sqrt[3]{w^3 + 4r_f^3} < r_f \cdot \sqrt[3]{\frac{8}{U_f}} \Rightarrow w^3 + 4r_f^3 < r_f^3 \frac{8}{U_f} \Rightarrow$$

$$\left(\frac{\sqrt{3}}{2} r_f \cdot \sqrt[3]{\frac{4\pi}{3U_f}}\right)^3 + 4r_f^3 < r_f^3 \frac{8}{U_f} \Rightarrow U_f < 2 - \frac{\pi\sqrt{3}}{8} \Rightarrow$$

$$U_f < 1.31982 \quad (25b)$$

Second Model:

$$a > 0 \Rightarrow \sqrt[3]{w^3 - 6r_f^3} > 0 \Rightarrow w^3 - 6r_f^3 > 0 \Rightarrow$$

$$\left(r_f \cdot \sqrt[3]{\frac{2\pi}{U_f}} \cdot \frac{\sqrt{2}}{2}\right)^3 - 6r_f^3 > 0 \Leftrightarrow r_f^3 \frac{2\pi}{U_f}\left(\frac{\sqrt{2}}{2}\right)^3 - 6r_f^3 > 0 \Rightarrow$$

$$U_f < \frac{\pi\sqrt{2}}{12} \Rightarrow U_f < 0.37024 \quad (25c)$$

$$b < c \Rightarrow \sqrt[3]{w^3 + 6r_f^3} < r_f \cdot \sqrt[3]{\frac{12}{U_f}} \Rightarrow w^3 + 6r_f^3 < r_f^3 \frac{12}{U_f} \Rightarrow$$

$$\left(\frac{\sqrt{2}}{2} r_f \cdot \sqrt[3]{\frac{2\pi}{U_f}}\right)^3 + 6r_f^3 < r_f^3 \frac{12}{U_f} \Rightarrow r_f^3 \frac{2\pi}{U_f}\left(\frac{\sqrt{2}}{2}\right)^3 + 6r_f^3 < r_f^3 \frac{12}{U_f} \Rightarrow$$

$$U_f < 2 - \frac{\pi\sqrt{3}}{8} \Rightarrow U_f < 1.31982 \quad (25d)$$

Third Model:

$$a > 0 \Rightarrow \sqrt[3]{w^3 - 3r_f^3} > 0 \Rightarrow w^3 - 3r_f^3 > 0 \Rightarrow$$

$$\left(\frac{1}{2} r_f \cdot \sqrt[3]{\frac{\pi}{U_f}}\right)^3 - 3r_f^3 > 0 \Leftrightarrow \frac{1}{8} r_f^3 \frac{\pi}{U_f} - 3r_f^3 > 0 \Rightarrow$$

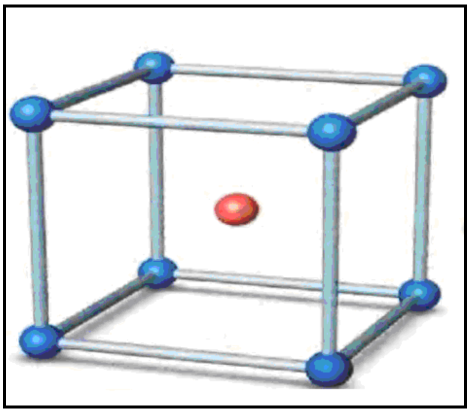
$$U_f < \frac{\pi}{24} \Rightarrow U_f < 0.13089 \quad (25e)$$

$$b < c \Rightarrow \sqrt[3]{w^3 + 3r_f^3} < r_f \cdot \sqrt[3]{\frac{12}{U_f}} \Rightarrow w^3 + 3r_f^3 < r_f^3 \frac{6}{U_f} \Rightarrow$$

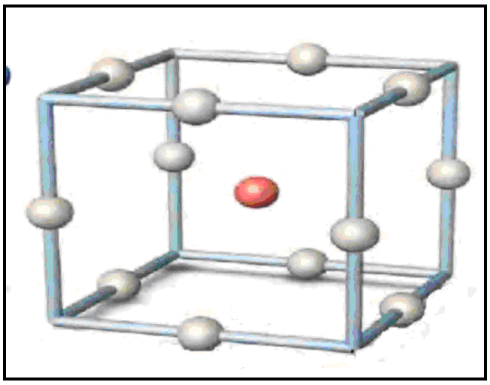
$$\left(\frac{1}{2} r_f \cdot \sqrt[3]{\frac{\pi}{U_f}}\right)^3 + 3r_f^3 < r_f^3 \frac{6}{U_f} \Rightarrow \frac{1}{8} r_f^3 \frac{\pi}{U_f} + 3r_f^3 < r_f^3 \frac{6}{U_f} \Rightarrow$$

$$U_f < 2 - \frac{\pi}{24} \Rightarrow U_f < 1.86910 \quad (25f)$$

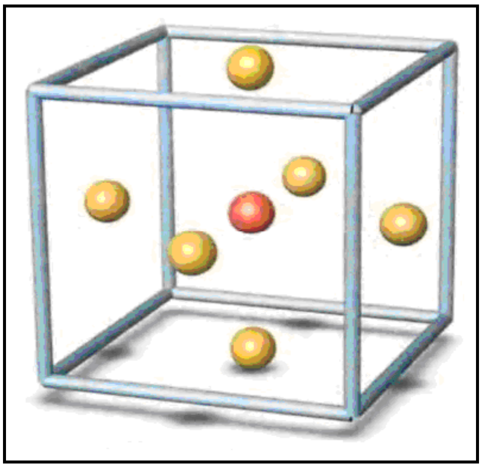
Alongside the above concept, the model adopted in Fig. 3 also represents a three – dimensional system capable of simulating real particulate composites. It performs a three-dimensional system capable of simulating real particle composites. Assuming equal fillers, which is not necessarily always the case, the volume fraction U_f, of the fillers in the continuous matrix is given in terms of the ratio $2r_f / \ell$ where r_f, is the filler radius and ℓ the side of the cube. Thus, we assume that a spherical inclusion lies at the centre of a cube whereas the neighbouring inclusions occupy the eight vertices of this cube or they are placed at the middle of each one of the twelve sides [Fig. 3], or finally they are placed at the centre of each one of the six faces.



IM$_1$



IM$_2$



IM$_3$

Fig. 3 (a,b,c) Interrelated tetraphase microstructural model

Next, we assume that a cube of side 2ℓ surrounding that of side ℓ constitutes the representative element. Thus we have the three variations M$_1$, M$_2$, M$_3$, respectively. And this array continues in all material as in Fig.2 for M$_1$. Now, in order to facilitate the analysis, we transform the cubic volume element to a spherical one according to the following assumptions, given that the volume fraction U_f and the radius r_f of the inclusions are known.

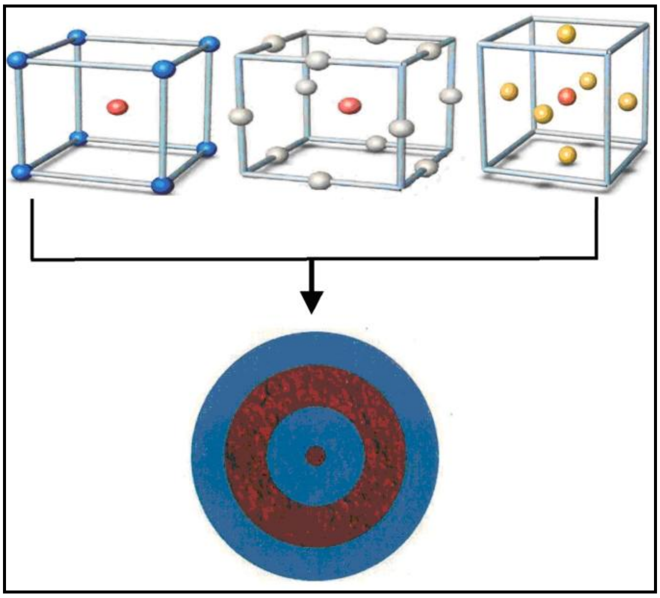


Fig. 4 Transformation of the tetraphase model

a. A sphere with radius d having equal volume with the cube of side 2ℓ.

b. A concentric sphere of radius $r_f = a$ which represents the central spherical inclusion.

c. A concentric hollow sphere of radii a and b which simulates the matrix between the central inclusion and the neighboring inclusions.

d. A concentric hollow sphere of radii b and c which simulates the neighboring inclusions and whose volume is equal to the volume of these inclusions. This zone represents the influence of other particles.

e. A concentric hollow sphere of radii c and d which simulates the remaining matrix that extends up to the vertices of the cube of side 2ℓ. The following relationships can be written in order to calculate the radii a, b, c and d:

The total volume fraction of the spheres in the cubic RVE is given as:

$$U_f = \frac{\frac{4}{3}\pi \cdot r_f^3 + N_i\left(\frac{4}{3}\pi \cdot r_f^3\right)}{(2\ell)^3} \Rightarrow$$

$$U_f = \frac{\frac{4}{3}(1+N_i)\pi \cdot r_f^3}{(2\ell)^3} \Rightarrow$$

$$\ell = r_f \cdot \sqrt[3]{\frac{(1+N_i)\pi}{6U_f}} \qquad (26)$$

where $N_i = 8$ or 12 or 6 and denotes the spheres in the cube for each variation M$_1$, M$_2$, M$_3$, of the present model respectively. The volume of the external cube with side 2 ℓ is equal to the volume of outer sphere with radius d

$$(2\ell)^3 = \frac{4}{3}\pi \cdot d^3 \Rightarrow$$

$$d = \ell \cdot \sqrt[3]{\frac{6}{\pi}} \qquad (27)$$

Eqns. (26), (27) yield

$$d = r_f \cdot \sqrt[3]{\frac{1+N_i}{U_f}} \qquad (28)$$

Now, let us consider the cube of side ℓ. The length of its main diagonal is $\ell\sqrt{3}$ whereas the diagonal of each face of the cube is $\ell\sqrt{2}$. If we denote by *w* the distance from the centre of the cube to a vertex or to a mid-side of the cube or to a centre of its faces we have:

$$w = \frac{\ell\sqrt{3}}{2} \rightarrow w_1$$

$$w = \frac{\ell\sqrt{2}}{2} \rightarrow w_2$$

$$w = \frac{\ell}{2} \rightarrow w_3 \qquad (29)$$

for M_1, M_2, M_3, respectively.
We consider that the volume of the hollow spherical region with radii *b* and *c* is distributed in equal parts of volume on both sides of the spherical surface of radius *w*.
Thus it follows

$$\frac{4}{3}\pi(c^3 - w^3) = \frac{4}{3}\pi(w^3 - b^3) \Rightarrow$$

$$c^3 + b^3 = 2w^3 \qquad (30)$$

The volume, however, of this region is equal to the volume of the eight, or twelve or six spherical inclusions depending on each one of the adopted variations M_1, M_2, M_3 of the model. Thus:

$$\frac{4}{3}\pi(c^3 - b^3) = \frac{4}{3}\pi \cdot r_f^3 \cdot N_i \Rightarrow$$

$$c^3 - b^3 = N_i \cdot r_f^3 \qquad (31)$$

where again $N_i = 8$ or 12 or 16 for M_1, M_2, M_3 respectively.
The solutions of Eqns. (30) and (31) for b and c yield:

$$b = \sqrt[3]{w^3 - \frac{N_i}{2} r_f^3}$$

$$c = b = \sqrt[3]{w^3 + \frac{N_i}{2} r_f^3} \qquad (32)$$

For M_1, M_2, M_3 respectively.
Next, let us try to verify whether these values are consistent as limit values of the filler content in each case since radius b must be positive and superior to radius a
For M_1:

$$\text{b>0} \rightarrow w^3 - 4r_f^3 > 0 \Rightarrow \left(\frac{\sqrt{3}}{2}\right)^3 \frac{9\pi}{6U_f} \cdot r_f^3 - 4r_f^3 \Rightarrow$$

$$U_f < 0.765 \qquad (33)$$

$$\text{a} < \text{b} \Rightarrow \text{a}^3 < \text{b}^3 \Rightarrow r_f^3 < w^3 - 4r_f^3 \Rightarrow$$

$$r_f^3 < \left(\frac{\sqrt{3}}{2}\right)^3 \frac{9\pi}{6U_f} \cdot r_f^3 - 4r_f^3 \Rightarrow$$

$$U_f < 0.612 \qquad (34)$$

Hence $U_{f\,\min} = 0{,}612$
For M_2:

$$\text{b >0} \Rightarrow w^3 - 6r_f^3 > 0 \Rightarrow \left(\frac{\sqrt{2}}{2}\right)^3 \frac{13\pi}{6U_f} \cdot r_f^3 - 6r_f^3 > 0 \Rightarrow$$

$$U_f < 0.344 \qquad (35)$$

Hence it implies that $U_{f\,\min} = 0{,}344$
For M_3:

$$\text{b>0} \Rightarrow w^3 - 3r_f^3 > 0 \Rightarrow \left(\frac{1}{2}\right)^3 \frac{7\pi}{6U_f} \cdot r_f^3 - 3r_f^3 > 0 \Rightarrow$$

$$U_f < 0.153 \qquad (36)$$

$$\text{a} < \text{b} \Rightarrow \text{a}^3 < \text{b}^3 \Rightarrow r_f^3 < (w^3 - 3r_f^3)$$

$$\Rightarrow r_f^3 < \left(\frac{1}{2}\right)^3 \frac{7\pi}{6U_f} \cdot r_f^3 - 3r_f^3 \Rightarrow$$

$$U_f < 0.115 \qquad (37)$$

Qualitative estimation of thermal conductivity coefficient
Let $u(r,\theta,t)$ be the temperature due to heat conduction, in polar coordinates, of the possible RVEs as it can be seen in Fig. 5a, b

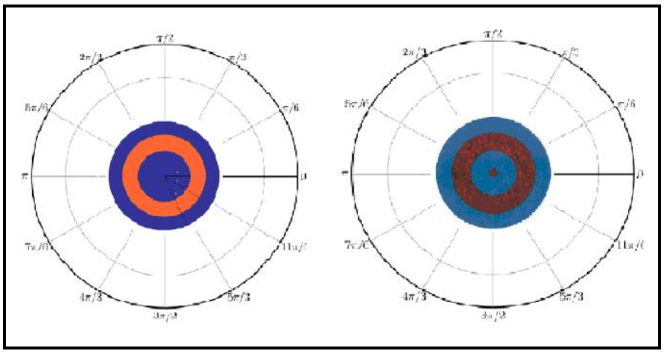


Fig. 5 a, b Propagation of heat through the possible RVEs of the composite

Then, the equation of propagation of heat (heat conduction) is written as

$$\frac{\partial u(r,\theta,t)}{\partial t}=\frac{K}{c\cdot\rho}\left(\frac{\partial^2 u(r,\theta,t)}{\partial r^2}+\frac{1}{r}\frac{\partial u(r,\theta,t)}{\partial r}+\frac{1}{r^2}\frac{\partial^2 u(r,\theta,t)}{\partial\theta^2}\right) \quad (38)$$

To be in accordance with the initial assumption that the particles are insulated, one should put the following boundary conditions

$$u(a,\theta,t)=ct;u(b,\theta,t)=ct;u(c,\theta,t)=ct \quad (39)$$

Moreover, without violating our proposed mathematical formalism let as also put the following initial condition

$$u(a,\theta,0)=f(r) \quad (40)$$

Next, we can point out that due the evident symmetry of the investigated problem the multi – valued function $u(r,\theta,t)$ does not depend on the variable θ and therefore eqn. (38) reduces to

$$\frac{\partial u(r,t)}{\partial t}=\frac{K}{c\cdot\rho}\left(\frac{\partial^2 u(r,t)}{\partial r^2}+\frac{1}{r}\frac{\partial u(r,t)}{\partial r}\right) \quad (41)$$

Let us try a solution in the form

$$u(r,t)=R(r)\cdot T(t) \quad (42)$$

Eqns. (39) and (40) can be combined to yield

$$\frac{1}{R}\cdot\frac{d^2R(r)}{dr^2}+\frac{1}{r}\frac{dR(r)}{dr}=\left(\frac{c\cdot\rho}{K}\right)\cdot\frac{dT(t)}{\partial t} \quad (43)$$

and therefore

$$\left(\frac{c\cdot\rho}{K}\right)\cdot\frac{1}{T(t)}\cdot\frac{dT(t)}{dt}=c_1 \quad (44)$$

$$\frac{1}{R}\cdot\frac{d^2R(r)}{dr^2}+\frac{1}{r}\cdot\frac{1}{R(r)}\cdot\frac{dR(r)}{dr}=c_1 \quad (45)$$

or equivalently

$$\frac{dT(t)}{dt}-\left(\frac{K}{c\cdot\rho}\right)\cdot c_1\cdot T(t)=0 \quad (46)$$

$$r\frac{d^2R(r)}{dr^2}+\frac{dR(r)}{dr}-c_1\cdot r\cdot R(r)=0 \quad (47)$$

The general solution of eqn. (44) is the following

$$T(t)=A'\cdot e^{c_1\frac{K}{c\cdot\rho}t} \quad (48)$$

Since the quantity $T(t)$ should always have finite values, even if the variable t tends to infinity, it implies that the arbitrary constant c_1 should be strictly negative. Thus eqn. (46) can be equivalently written as

$$T(t)=A'\cdot e^{-\lambda^2\cdot\frac{K}{c\cdot\rho}t} \quad (49)$$

Hence by substituting the auxiliary variable $-\lambda^2=c_1$ back into eqn. (45) we infer

$$r\frac{d^2R(r)}{dr^2}+\frac{dR(r)}{dr}+\lambda^2\cdot r\cdot R(r)=0\Rightarrow$$

$$r^2\frac{d^2R(r)}{dr^2}+r\frac{dR(r)}{dr}+\lambda^2\cdot r^2\cdot R(r)=0 \quad (50)$$

The generic form of the above ordinary differential equation is

$$r^2\frac{d^2R(r)}{dr^2}+r\frac{dR(r)}{dr}+(\lambda^2\cdot r^2-m^2)\cdot R(r)=0 \quad (51)$$

with $m=0$

Evidently, eqn. (51) is a Bessel equation of order zero, the general solution of which reads

$$R(r)=B'J_0(\lambda r)+C'\,Y_0(\lambda r) \quad (52)$$

where J_0 and Y_0 are the Bessel Functions of first and second kind, order zero, respectively.

Consequently, the general solution of eqn. (41), by the aid of eqn. (42) is represented as follows

$$u(r,t)=A'\cdot e^{-\lambda^2\cdot\frac{K}{c\cdot\rho}t}(B'\cdot J_0(\lambda r)+C'\cdot Y_0(\lambda r))\Leftrightarrow$$

$$u(r,t)=e^{-\lambda^2\cdot\frac{K}{c\cdot\rho}t}(A\cdot J_0(\lambda r)+B\cdot Y_0(\lambda r)) \quad (53)$$

with $A=A'\cdot B';B=A'\cdot C'$

Apparently, at $r=0$ the term $Y_0(\lambda r)$ tends to infinity, therefore since the temperature $u(r,t)$ is a finite quantity, one should request beforehand that $B=0$. Thus eqn. (53) yields

$$u(r,t)=A\cdot J_0(\lambda r)\cdot e^{-\lambda^2\cdot\frac{K}{c\cdot\rho}t}\Leftrightarrow$$

$$u(r,t)=A\cdot e^{-\lambda^2\cdot\frac{K}{c\cdot\rho}t}\cdot\sum_{n=0}^{\infty}\frac{(-1)^n}{(n!)^2}\left(\frac{\lambda r}{2}\right)^{2n} \quad (54)$$

The right member of eqn. (54) constitutes a particular integral of eqn. (41). Here, we should remark that according to our initial assumption, the particles inside the matrix are insulated and therefore the thermal conductivity of them is zero. This implies that the previously mentioned geometrical models for the particle contiguity contain at least one impenetrable layer. Hence, taking into account the boundary conditions one finds

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n!)^2}\left(\frac{\lambda a}{2}\right)^{2n}=C_1 \quad (55)$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n!)^2}\left(\frac{\lambda b}{2}\right)^{2n}=C_2 \quad (56)$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n!)^2}\left(\frac{\lambda c}{2}\right)^{2n}=C_3 \quad (57)$$

Thus, the derivative of Bessel Function of first kind, order zero, should vanish for λa ; λb ; λc respectively that is

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n-1)!n!}\left(\frac{\lambda a}{2}\right)^{2n-1}=0 \quad (58)$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n-1)!n!}\left(\frac{\lambda b}{2}\right)^{2n-1}=0 \quad (59)$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n-1)!n!}\left(\frac{\lambda c}{2}\right)^{2n-1}=0 \quad (60)$$

The positive roots $S_{0\,(n)}$ of the above equation can be determined by means of several methods [16, 17].
Thus it follows,

$$\lambda = \frac{S_{0\,(n)}}{a} \vee \lambda = \frac{S_{0\,(n)}}{b} \vee \lambda = \frac{S_{0\,(n)}}{c} \qquad (61)$$

Hence, with the exception of the impenetrable layer, we infer

$$u(r,t) = \sum_{n=1}^{+\infty} A_n \cdot e^{-\left(\frac{S_{0\,(n)}}{a}\right)^2 \cdot \frac{K}{c\cdot\rho} t} \cdot \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{\frac{S_{0\,(n)}}{a} r}{2} \right)^{2n} \qquad (62)$$

with $r \in [0, c-b+a]$ or $r \in (0, c-b+a]$ for the models illustrated in Figs. 5 a, and 5b respectively. Also, the term A_n can be calculated by the initial condition, i.e. eqn. (40), for both cases. Specifically, the single – valued function $f(r)$ appearing in eqn. (40) is expressed as power series of Bessel functions of the first kind, first and zero order. Hence, the above expression can lead after all to a qualitative evaluation of thermal conductivity coefficient given that the heat capacity and density of the composite are known.

Discussion

In this investigation, the authors dealt with a qualitative evaluation of the thermal conductivity coefficient for a large category of polymer periodic composites, reinforced with insulated spherical particles. In general, such materials are macroscopically considered as homogeneous. The two microstructural models that we adopted here to simulate the particle contiguity as well as a possible effect of the interaction amongst the particles have as their basic cell a three – phase and a four – phase spherical Representative Volume Element, respectively. Such geometrical models are generally characterized as reliable and indeed have good prospects. The analytical treatment that we proposed here has its basis in the closed – form solution of the partial deferential equation of unsteady state heat conduction for a two dimensional simply – connected compound disk. Evidently, this means that an arbitrary simply – closed curve which lies throughout in this compact region can be shrunk to any point without leaving the region, even if this point belongs to the impenetrable rings of Figs. (5 a,b) or coincides with the impenetrable centre of the disk as it can be observed in Fig. 5b. Moreover, the application of this mathematical method, premises that the heat capacity and the density of the composite are given, or they can be expressed with respect to the filler content, taking into account the restrictions that we have already formulated concerning these aforementioned geometrical models. Hence, provided that the change of temperature of the overall material is able to be measured for distinct time values, one may obtain a qualitative estimation of the thermal conductivity of the composite.

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