

MODELS OF EFFECTIVE THERMAL CONDUCTIVITY OF BINARY COMPOSITE SYSTEMS

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Abstract. Methods for calculating the physical properties (thermal conductivity) of composite materials (CS) based on empirical and numerical models are investigated. These use the idea of Maxwell and Rayleigh about the proportionality of this parameter to the physical properties of the matrix and filler, as well as the concentration of the filler in the matrix. These models can consider the shape of the particles and their relative position. Comparison experimental data showed that such models are not universal and work only in the field of low concentrations of filler in the matrix. Another class of effective thermal conductivity models allows you to consider Thermal boundary resistance of the contact between the filler particles and the matrix (Kapitza thermal resistance). In this case, there is a serious problem of determining the thickness of the interfacial thermal layer, which can only be estimated by indirect methods. In general, the effective thermal conductivity of the composite (ETC) is also influenced by other factors: contact thermal resistance between filler particles, aggregation of filler particles, dependence of the physical properties of the filler on particle size, ordering of matrix molecules in the interfacial region. Numerical calculation is the most efficient because it is possible to consider the influence of a lot of factors, which is not possible in the case of an empirical model. A composite is a heterogeneous structure, so the generalized heat flux method is applicable. The average heat flux through the composite is calculated and then the effective thermal conductivity coefficient of the composite is calculated. The calculation of ETC is performed using the generalized heat flux method (GHFM). To solve the transient thermal conductivity equation, the Alternating Direction Implicit Method (ADI) was used. Methods for estimating the thickness of the Thermal boundary are proposed based on comparison of experimental data and the results of a computational experiment and considering the dimensional factor. The concentrations of the filler at which these factors have the greatest effect on the thermal conductivity of the composite have been determined. Software has been developed by applying the methods described.

Keywords: effective thermal conductivity, analytical models, numerical simulation, finite element analysis.

1. INTRODUCTION

The development of computational methods for effective thermal conductivity of composite systems was based on intuitively understandable dependencies of thermal conductivity on the concentration of the filler in the matrix, on the distribution of particles in the matrix, the geometry and orientation of the particles, the ratio of the thermal conductivity coefficients of the matrix and the filler, the clustering of filler particles, the ratio of particle sizes and the CS object, the interfacial thermal resistance (Kapitza resistance), and the contact thermal resistances between particles in a cluster. In general, this dependence can be represented by the expression [1].

$$\frac{\lambda_{eff}}{\lambda_1} = f\left(\frac{\lambda_2}{\lambda_1}, \rho_2, \frac{a}{L}, Bi\right) \quad (1)$$

λ_{eff} – ETC; λ_1 – thermal conductivity coefficient of the matrix; λ_2 – Thermal conductivity coefficient of the filler; ρ_2 – Bulk concentration of filler; a – Particle Radius; Bio Number $Bi = a/R_c\lambda_2$; L – Object size.

Let us consider the influence of these factors on ETC. In the field of our consideration will be polymer composites with a filler that has a higher thermal conductivity coefficient than the matrix. Such composites are in demand in systems where energy removal (cooling) is relevant, for example, electronic devices. The range of changes in the thermal conductivity coefficient of polymers used as a matrix is quite narrow from 0.1 to 0.4 W/(m·K). The range the coefficient of thermal conductivity of the filler is from 0.8 to 3000 W/(m·K). The task comes down to the need to obtain the maximum effective coefficient of thermal conductivity at specified materials of the matrix and filler. It is not easy to solve this problem experimentally, due to the influence of large number of factors including. The use of thermal conductivity modeling of a composite system can significantly speed up the process of creating a material with desired properties.

2. EMPIRICAL METHODS

Let's start with a review of empirical methods based on the Maxwell-Rayleigh model [2, 3]. Maxwell's model contains only the bulk concentrations and the thermal conductivity of the matrix and the filler, respectively, does not consider the structure of the filler, interfacial and contact thermal resistance, so it can only be used for preliminary estimates of the effective coefficient of thermal conductivity:

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{3\rho_2}{\frac{(\lambda_2 + 2\lambda_1)}{\lambda_2 - \lambda_1} - \rho_2} \right), \quad (2)$$

Rayleigh's model [3] considers the shape of the filler particles and their orientation: for spherical particles,

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{3\rho_2}{\frac{(\lambda_2 - 2\lambda_1)}{\lambda_2 - \lambda_1} - \rho_2 + \frac{1.569((\lambda_2 - \lambda_1))}{(3\lambda_2 - 4\lambda_1)} \rho_2^{3.33}} \right) \quad (3)$$

cylindrical particles located across the heat flow,

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{2\rho_2}{\frac{(\lambda_2 + \lambda_1)}{\lambda_2 - \lambda_1} - \rho_2 + \frac{(\lambda_2 - \lambda_1)}{(\lambda_2 - \lambda_1)(0.3058\rho_2^4 + 0.01336\rho_2^8)}} \right) \quad (4)$$

cylindrical particles located along the heat flow,

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{(\lambda_2 - \lambda_1)\rho_2}{\lambda_1} \right) \quad (5)$$

The Maxwell–Eucken model orients particles in the form of spheroids, cylinders, and plates:

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{(\lambda_2/\lambda_1 - 1)L\rho_2}{1 + (L - 1)\rho_2} \right). \quad (6)$$

For spheroids ($f_1 = f_2 \neq f_3$), $L = \frac{1}{3} \sum_{i=1}^3 \left[1 + \left(\frac{\lambda_2}{\lambda_1} - 1 \right) f_i \right]^{-1}$, $\sum_{i=1}^3 f_i = 1$,

here are the semi-axes of the ellipsoid, f_i $L = (5\lambda_1 + \lambda_2)/[3(\lambda_1 + \lambda_2)]$ for the cylindrical shape of the filler particles, for the spherical shape of the filler particles; – for the lamellar form of filler particles. $L = 3\lambda_1/(2\lambda_1 + \lambda_2)$ $L = (\lambda_1 + 2\lambda_2)/3\lambda_1$

Fig.1 (2) plots relationships (2), (3), (6) and shows experimental data for ETC with an epoxy resin matrix at bulk concentrations less than 0.1. As demonstrated, the ETC remains virtually unchanged across different filler materials because of the absence of particle clusters. Consequently, the thermal conductivity of the matrix remains the primary controlling factor. This range is well described by models (3), (4), (6). Fig.1 (2) indicates that other models are needed for high concentrations of filler. Experimental data taken from [4, 5].

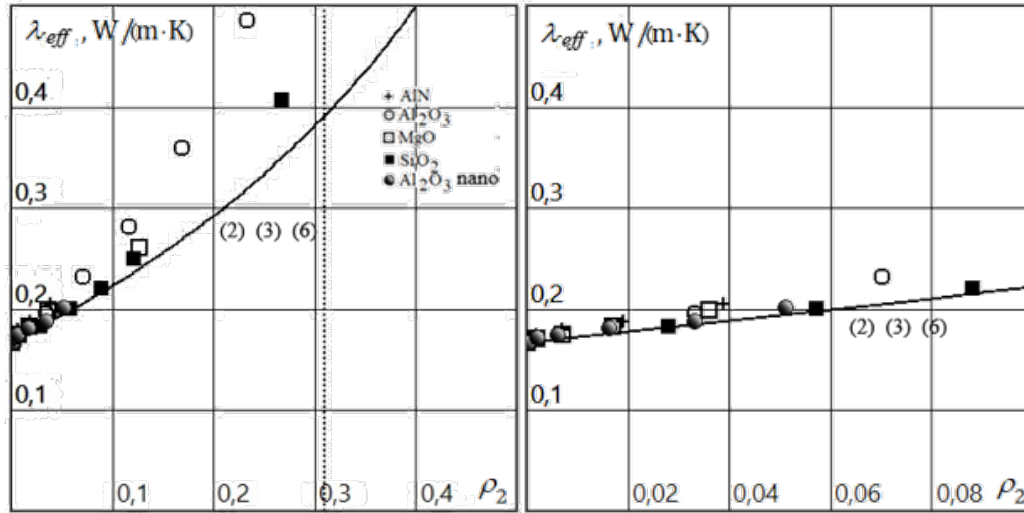


Figure 1 – ETC. The matrix is made of epoxy resin. 1. High concentrations of filler. 2. Low concentration of filler.

We consider two additional models to calculate the effective thermal conductivity coefficient, based solely on the filler volume fraction and the thermal conductivity of the matrix. The first is Odelevsky's model [6]:

$$\lambda_{\text{eff}} = \left(\frac{(3\rho_1 - 1)\lambda_1 + (3\rho_2 - 1)\lambda_2}{4} \right) + \left[\left(\frac{(3\rho_1 - 1)\lambda_1 + (3\rho_2 - 1)\lambda_2}{4} \right)^2 + \frac{\lambda_1\lambda_2}{2} \right]^{0.5}, \quad (7)$$

Lewis-Nielsen model [3]:

$$\lambda_{\text{eff}} = \lambda_1 \frac{1 + AB\rho_2}{1 - B\rho_2\psi} \quad (8)$$

$$B = \frac{\frac{\lambda_2}{\lambda_1} - 1}{\frac{\lambda_2}{\lambda_1} + A}; \quad \psi = 1 + \frac{1 - \rho_{2m}}{\rho_{2m}^2} \rho_2,$$

where A is the particle shape coefficient (1.5 – sphere), ρ_{2m} is the maximum particle packing (0.52).

As shown in Figure 2, the models align closely with the experimental data for aluminum oxide and silicon dioxide fillers, even at high concentrations. However, this agreement may be coincidental, given the lack of clear criteria to compare calculated and experimental values. Furthermore, exact experimental conditions are not always specified. The thermal conductivity of silicon dioxide, for example, can range from 0.02 to 10 W/(m·K) depending on its structural state. The experimental data are labeled as in Fig.1 (1). The considered models use the concentrations and thermal conductivities of the composite components as parameters. A more advanced approach is the Hasselman-Johnson

calculation method [7]. This account for the thermal resistance of the interfacial layer. For a spherical particle, the formula is:

$$\lambda_{eff} = \lambda_1 \frac{\left[2 \left(\frac{\lambda_2}{\lambda_1} - \frac{\lambda_2}{ah_c} - 1 \right) \rho_2 + \frac{\lambda_2}{\lambda_1} + \frac{2\lambda_2}{ah_c} + 2 \right]}{\left[\left(1 - \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} \right) \rho_2 + \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} + 2 \right]}, \quad (9)$$

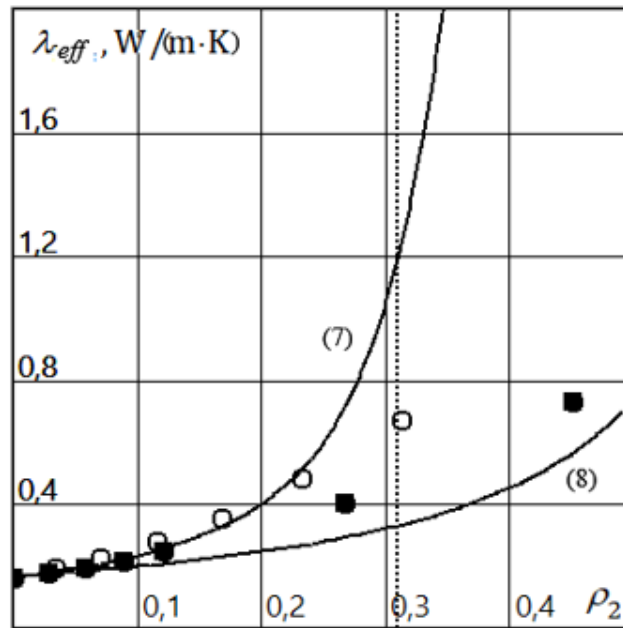


Figure 2 – Effective thermal conductivity of the epoxy-based composite. The solid lines represent the theoretical predictions by the Odelevsky (7) and Lewis-Nielsen models (8).

cylindrical,

$$\lambda_{eff} = \lambda_1 \frac{\left[\left(\frac{\lambda_2}{\lambda_1} - \frac{\lambda_2}{ah_c} - 1 \right) \rho_2 + \frac{\lambda_2}{\lambda_1} + \frac{2\lambda_2}{ah_c} + 1 \right]}{\left[\left(1 - \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} \right) \rho_2 - \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} + 1 \right]} \quad (10)$$

plate,

$$\lambda_{eff} = \lambda_1 \frac{1}{\left[\left(1 - \frac{\lambda_2}{\lambda_1} + \frac{2\lambda_2}{ah_c} \right) \rho_2 + \frac{\lambda_2}{\lambda_1} \right]} \quad (11)$$

The Every and Tzou model belongs to the same category of models [3]:

$$(1 - \rho_2)^3 = \left(\frac{\lambda_1}{\lambda_{eff}} \right)^{(1+2\alpha)/(1-\alpha)} \left(\frac{\lambda_{eff} - \lambda_2(1-\alpha)}{\lambda_1 - \lambda_2(1-\alpha)} \right)^{3/(1-\alpha)} \quad (12)$$

where α – a coefficient that consider the particle size and interfacial thermal resistance, $\alpha = 2a_K/d$, where $a_K = \lambda_1/h_c$ is the Kapitza radius.

Fig.3 illustrates the empirical relationships of the equivalent thermal conductivity (ETC) for epoxy resin composites filled with aluminum oxide. Analyses of Figures 2 and 3 reveal that the Odelevsky and Hasselmann-Johnson models provide the best fit. However, these models differ significantly: the Odelevsky model relies solely on filler concentration, whereas the Hasselmann-Johnson model incorporates the properties of the interfacial layer. Estimates indicate that the thickness of the Kapitza

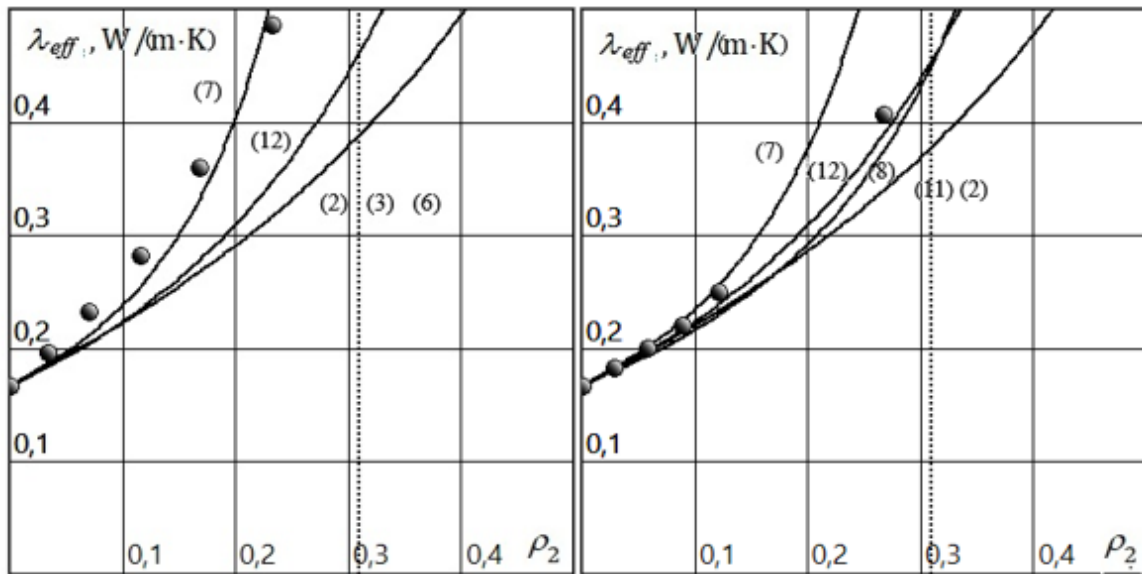


Figure 3 – Epoxy resin matrix with different fillers: 1) aluminum oxide (particle size of 4 μm); 2) silicon dioxide (particle size of 20 μm).

(interfacial) layer ranges from 2 to 16 nm [4], with the thermal boundary conductance of this layer reaching $10^8 \text{ W}/(\text{m}^2 \cdot \text{K})$.

Fig.4 presents a comparison between the experimental findings and the empirical models for the polyethylene–SiC and polyamide–SiC composites.

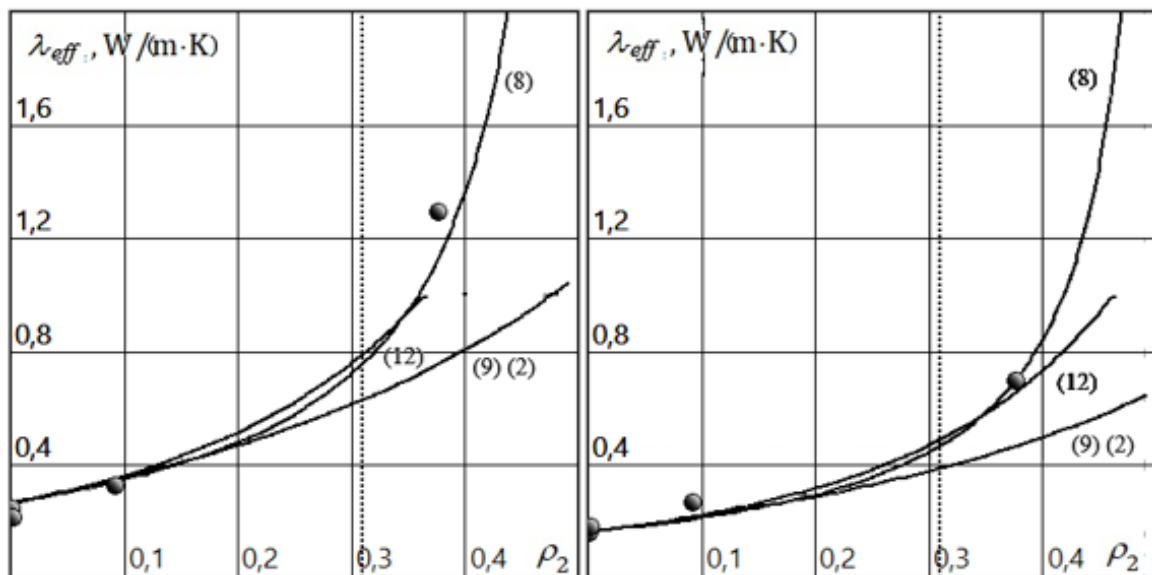


Figure 4 – 1) Polyamide–silicon carbide; 2) Polyethylene–silicon carbide; particle size 1 μm).

These models properly account for the interfacial thermal resistance. Nonetheless, the fundamental physics of energy transport at this interface requires further investigation.

Another frequently used model is the percolation model [8]:

$$\lambda_{\text{eff}} = \lambda_2 \left(\frac{\rho_1 - \rho_c}{1 - \rho_c} \right)^k, \quad (13)$$

$$\lambda_{\text{eff}} = \lambda_2 \left(\frac{\lambda_c}{\lambda_2} \right)^{\left(\frac{1-\rho_2}{1-\rho_c} \right)^k} \quad (14)$$

$k = 1.6, \rho_c = 0.15$.

This model includes a clustering parameter, ρ_c , which describes how particles clump together. In chaotic systems, particle clusters always form, causing contact resistance to add to interfacial resistance. At a volume concentration of roughly 0.311, a continuous chain of filler particles (a percolation cluster) forms, which dramatically increases conductivity. While this effect is vital for conductive metal fillers, we focus on dielectric fillers and omit percolation models. In all figures, the vertical dotted line corresponds to the concentration of the filler at the percolation threshold.

Fig.5 and 6 show the relative errors in the ETC calculation for different empirical models. The figures indicate that a calculation error of less than 10% is achieved only at filler concentrations of 0.1 or lower. Comparisons of empirical methods show they are only valid for dilute filler concentrations and preliminary ETC estimates. To account for a maximum number of influencing factors, numerical models must be used.

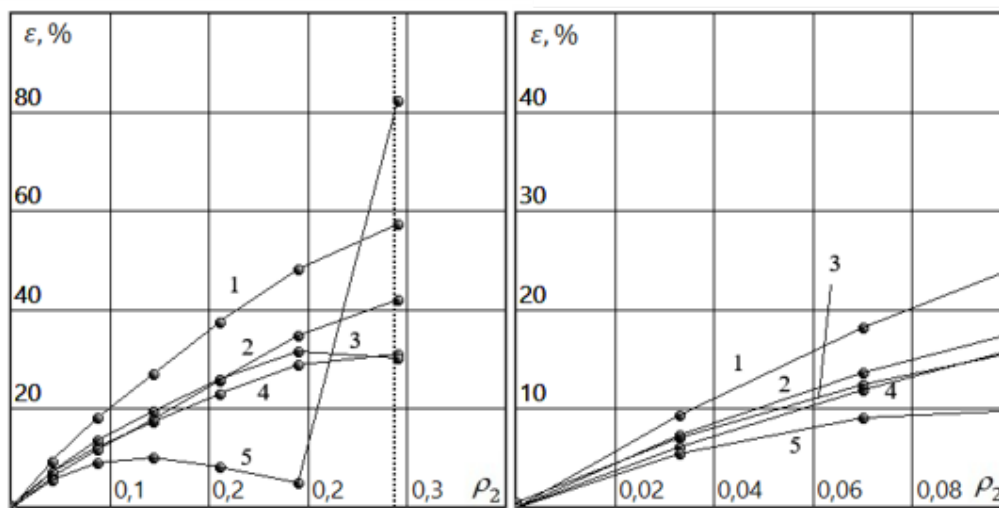


Figure 5 – Relative error of the thermal conductivity coefficient for the epoxy resin matrix with aluminum oxide (particle size of 4 μm). 1. Hasselmann-Johnson 2. Maxwell-Rayleigh. 3. Lewis-Nielsen. 4. Every-Tzow 5. Odelevsky.

3. NUMERICAL METHODS

We solve the transient heat conduction equation to determine the temperature field for the GHFM:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda_z \frac{\partial T}{\partial z} \right), \quad (15)$$

x, y, z – coordinates, m; ρ – density, kg/m^3 ; C_p – heat capacity; t – time, s; T – temperature, λ – Thermal Conductivity Coefficient, $\text{W}/(\text{m} \cdot \text{K})$.

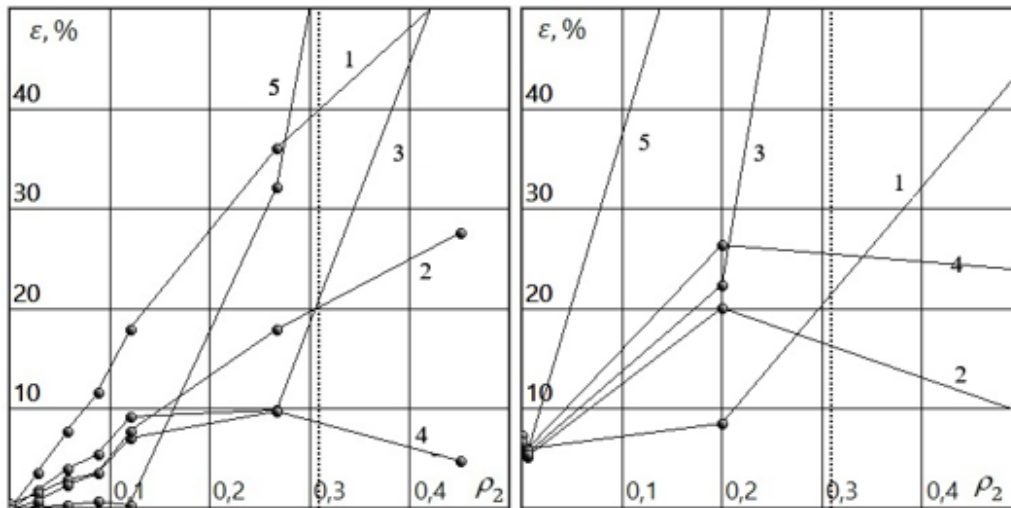


Figure 6 – Relative error in the effective thermal conductivity coefficient for (1) epoxy resin/SiO₂ (20 μm) and (2) polyamide/SiC (1 μm) composites. 1. Hasselmann-Johnson 2. Maxwell-Rayleigh. 3. Lewis-Nielsen. 4. Every-Tzow 5. Odelevsky.

The boundary conditions are shown (Fig. 7):

$$\begin{aligned}
 T &= T_b, \quad L_x \geq x \geq 0, \quad y = 0, \quad L_z \geq z \geq 0; \\
 T &= T_e, \quad L_x \geq x \geq 0, \quad y = L_y, \quad L_z \geq z \geq 0; \\
 T &= T_0, \quad L_x > x > 0, \quad L_y > y > 0, \quad L_z > z \geq 0; \\
 \frac{\partial T}{\partial x} &= 0, \quad \frac{\partial T}{\partial z} = 0, \quad x = 0, \quad x = L_x; \quad L_y > y > 0, \quad z = 0, \quad z = L_z,
 \end{aligned} \tag{16}$$

L_x, L_y, L_z – Linear dimensions of the element.

This problem was solved in [9, 10] by the relaxation method. In this work, the ADI (Alternating Direction Implicit) method of fractional steps is applied [11, 12]. The finite-difference representation of equation (15) is approximated by the unconditionally stable implicit scheme [13].

$$\rho C_p \frac{T_{ijk}^{n+1} - T_{ijk}^n}{\Delta t} = \sum_{m=i,j,k} \frac{\Theta [\delta(\lambda \delta T_{ijk})]_m^{n+1} + (1 - \Theta) [\delta(\lambda \delta T_{ijk})]_m^n}{(\Delta h)^2}, \tag{17}$$

where

$m = i, j, k$;

$i = 1 \dots N_x, j = 1 \dots N_y, k = 1 \dots N_z$;

$n = 0, 1, 2 \dots$ – time step index;

Δh – the step of splitting by coordinates (we assume the same along the x, y and z axes);

$0 \leq \Theta < 1$ – Weighting coefficient.

When $m = i$, the expression for $[\delta(\lambda \delta T_{ijk})]_i^{n+1}$ is written as:

$$[\delta(\lambda \delta T_{ijk})]_i^{n+1} = \lambda_{i+\frac{1}{2}} (T_{i+1,jk}^{n+1} - T_{ijk}^{n+1}) - \lambda_{i-\frac{1}{2}} (T_{ijk}^{n+1} - T_{i-1,jk}^{n+1}) \tag{18}$$

The system of equations (16) can be rewritten using matrix difference operators with variable coefficients considering (17):

$$T_{ijk}^{n+1} - T_{ijk}^n = \Theta (\Lambda_1 T^{n+1} + \Lambda_2 T^{n+1} + \Lambda_3 T^{n+1}) + (1 - \Theta) \Lambda_1 T^n + \Lambda_2 T^n + \Lambda_3 T^n \tag{19}$$

where $\Lambda_1, \Lambda_2, \Lambda_3$ – matrix difference operators with variable coefficients.
Apply these operators to the expression (19):

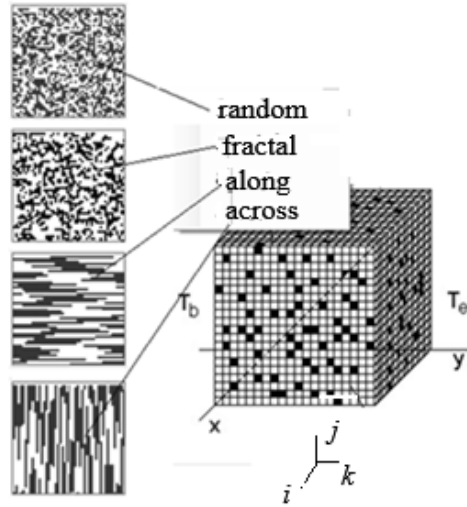


Figure 7 – On formulating a mathematical problem.

$$\Lambda_1 T^d = \text{Fo}_{i+1/2} T_{i+1,jk}^d - (\text{Fo}_{i+1/2} + \text{Fo}_{i-1/2}) T_{ijk}^d + \text{Fo}_{i-1/2} T_{i-1,jk}^d, \quad (20)$$

$$\Lambda_2 T^d = \text{Fo}_{j+1/2} T_{i,j+1,k}^d - (\text{Fo}_{j+1/2} + \text{Fo}_{j-1/2}) T_{ijk}^d + \text{Fo}_{j-1/2} T_{i,j-1,k}^d, \quad (21)$$

$$\Lambda_3 T^d = \text{Fo}_{k+1/2} T_{i,j,k+1}^d - (\text{Fo}_{k+1/2} + \text{Fo}_{k-1/2}) T_{ijk}^d + \text{Fo}_{k-1/2} T_{i,j,k-1}^d, \quad (22)$$

where $d = n + 1$ or $d = n$.

$1 \leq i \leq N_x, 1 \leq j \leq N_y, 1 \leq k \leq N_z$ – coordinates indices; Δt – time step, s; Δh – step by coordinates, m;

N_x, N_y, N_z – Number of nodes on the x, y, z axes. Fourier number:

$$\text{Fo}_{m+1/2} = \frac{\lambda_{m+1/2} \Delta t}{\rho C_p \Delta h^2}; \quad \text{Fo}_{i-1/2} = \frac{\lambda_{m-1/2} \Delta t}{\rho C_p \Delta h^2};$$

$$\lambda_{m\pm 1/2} = \frac{2}{\frac{1}{\lambda_{1(m\pm 1)}} + \frac{1}{\lambda_{2(m\pm 1)}} + \frac{2}{K_c \Delta h}} \quad \text{– particle-matrix contact,}$$

$$\lambda_{m\pm 1/2} = \frac{1}{\frac{1}{\lambda_{2(m\pm 1)}} + \frac{1}{K_p \Delta h}} \quad \text{– particle-to-particle contact,}$$

K_c – thermal conductivity of the particle-matrix contact (interfacial contact),

K_p – thermal conductivity of particle-to-particle contact.

$C_p = \frac{C_1 + C_2}{2}$ – Average heat capacity of contacting elements,

The system of equations (19) can be solved by the method of fractional steps [11, 12]. For this purpose, the time-step discretization is defined as follows:

$$-\Theta \Lambda_1 T^{n+1/3} + T_{ijk}^{n+1/3} = (1 - \Theta) \Lambda_1 T^n + T_{ijk}^n \quad (23)$$

$$-\Theta \Lambda_2 T^{n+2/3} + T_{ijk}^{n+2/3} = (1 - \Theta) \Lambda_2 T^{n+1/3} + T_{ijk}^{n+1/3} \quad (24)$$

$$-\Theta \Lambda_3 T^{n+1} + T_{ijk}^{n+1} = (1 - \Theta) \Lambda_3 T^{n+2/3} + T_{ijk}^{n+2/3}, \quad (25)$$

The main time step Δt is divided into three intervals: the index $n + 1/3$ corresponds to the moment in time $t_{n+1/3} = t_n + 1/3\Delta t$, $t_{n+2/3} = t_n + 2/3\Delta t$, $t_{n+1} = t_n + \Delta t$. Equations (23)–(25) are solvable at a single timestep via the forward-backward sweep method. The solution procedure is detailed below using equation (23) as an example. The tridiagonal matrix algorithm is applied. To proceed, group the terms associated with moments n and $n + 1/3$.

$$-\Theta(\text{Fo}_{i+1/2/3})T_{i+1,jk}^{n+1/3} + (1 + \Theta\text{Fo}_{i+1/2/3} + \Theta\text{Fo}_{i-1/2/3})T_{ijk}^{n+1/3} - \Theta T_{i-1,jk}^{n+1/3}\text{Fo}_{i-1/2/3} = G_i \quad (26)$$

$$G_i = (1 - \Theta)\Lambda_1 T^n + T_{ijk}^n.$$

Let's rewrite (26) considering the new designations:

$$A_i = \Theta(\text{Fo}_{i+1/2/3}); B_i = 1 + \Theta\text{Fo}_{i+1/2/3} + \Theta\text{Fo}_{i-1/2/3}; C_i = \Theta\text{Fo}_{i-1/2/3},$$

$$-A_i T_{i+1,jk}^{n+1/3} + B_i T_{ijk}^{n+1/3} - C_i T_{i-1,jk}^{n+1/3} = G_i \quad (27)$$

A solution to Equation (27) is sought in the form:

$$T_{ijk}^{n+1/3} = E_i T_{i+1,jk}^{n+1/3} + F_i \quad (28)$$

Replace in (27) $T_{i-1,jk}^{n+1/3}$ using expression (28), resulting in:

$$E_i = \frac{A_i}{B_i - C_i E_{i-1}} \quad (29)$$

$$F_i = \frac{G_i - C_i F_{i-1}}{B_i - C_i E_{i-1}} \quad (30)$$

From the boundary condition $i = 1$ where $\frac{\partial T}{\partial x} = 0$, we obtain:

$$E_0 = 1, \quad F_0 = 0 \quad (31)$$

Using (29)–(31), we can calculate by induction in the ascending direction E_i and F_i , and then from expression (27) we find the temperatures $T_{ijk}^{n+1/3}$. Equations (24) and (25) are solved in the same way. The only difference lies in the starting values of E_i F_i . From the boundary condition $k = 1$ where $T_{1,jk} = T_b$, we obtain:

$$E_0 = 0, \quad F_0 = T_b, \quad (32)$$

From the boundary condition $j = 1$ where $\frac{\partial T}{\partial z} = 0$, we obtain:

$$E_0 = 1, \quad F_0 = 0 \quad (33)$$

As a result, the temperatures in all nodes of the grid for the current time step will be obtained. Average heat flux through sample:

$$q_{avi} = \frac{1}{N_x(N_y - 1)N_z} \sum_{j=1}^{N_z} \sum_{k=1}^{N_y-1} \sum_{i=1}^{N_x} \lambda_{ij,k+1/2} \frac{(T_{ijk+1} - T_{ijk})}{\Delta h} \quad (34)$$

The effective thermal conductivity coefficient of the composite is calculated by the following equation:

$$\lambda_{eff} = \frac{q_{avi} \cdot L_x}{T_e - T_b} \quad (35)$$

The software was developed to implement equations (18)–(35). To verify the algorithm, we simulated the temperature distribution in a homogeneous sample under specific boundary conditions (16). The initial temperature distribution along the y-axis was assumed to be linear. Other parameters had the following values: time step $\Delta t = 10^{-6}$ s, coordinate step, temperature interval, thermal conductivity coefficient of the material, weight coefficient $\Delta h = 10^{-5}$ m, $T_e - T_b = 200$ K, $\lambda = 40$ W/(m·K), $\Theta = 0.5$ (Crank–Nicolson scheme), random distribution of the filler in the matrix. The remaining parameters were defined as follows: time step $\Delta t = 10^{-6}$ s, coordinate step $\Delta h = 10^{-5}$ m, temperature interval $T_e - T_b = 200$ K, thermal conductivity of the material = 40 W/(m·K) and weight coefficient $\Theta = 0.5$ (Crank–Nicolson scheme). The filler was assumed to be randomly distributed within the matrix. The thermal conductivity coefficient of the material was calculated $\lambda = 39.998$ W/(m·K), with the temperature determination error not exceeding 0.5%. Similar results were obtained using a purely implicit scheme, where $\Theta = 1$.

The composite structure is generated on a volumetric lattice with dimensions $L_x \times L_y \times L_z$. After setting the volumetric concentration of the filler, the number of cells per filler particle is calculated. The required distribution of the filler within the matrix is then generated (Fig. 7). Figure 8 presents the numerical calculations and compares them with experimental data regarding the effective thermal conductivity coefficient. The value of interfacial thermal resistance $R_c = 1/K_c$ was determined by expression (40). The thermal resistance of the particle-to-particle contact $R_p = 1/K_p$,

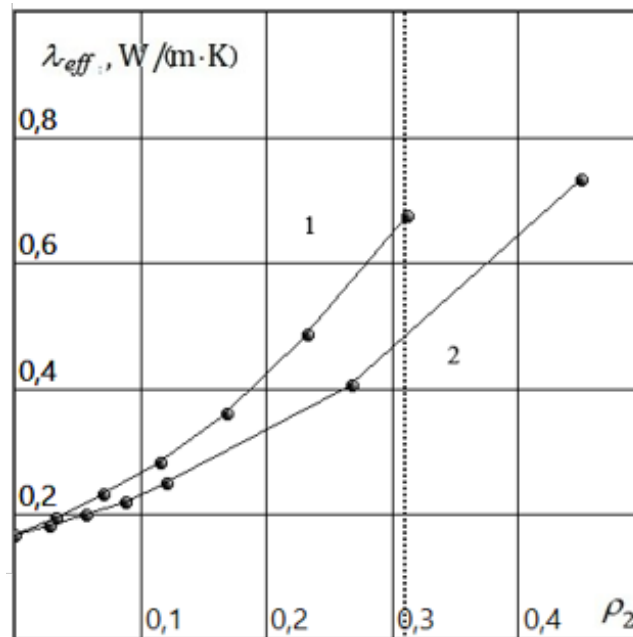


Figure 8 – Epoxy resin matrix: 1. aluminum oxide (particle size of 4 μm); 2. silicon dioxide (particle size of 20 μm); Points – experiment, lines – numerical calculations.

The developed software enables the generation of various filler distributions within the matrix (Fig. 7). The influence of these distributions on the effective thermal conductivity (ETC) is depicted in Fig. 8.

Next, we will briefly discuss the factors that complicate the calculation of thermal conductivity in composites.

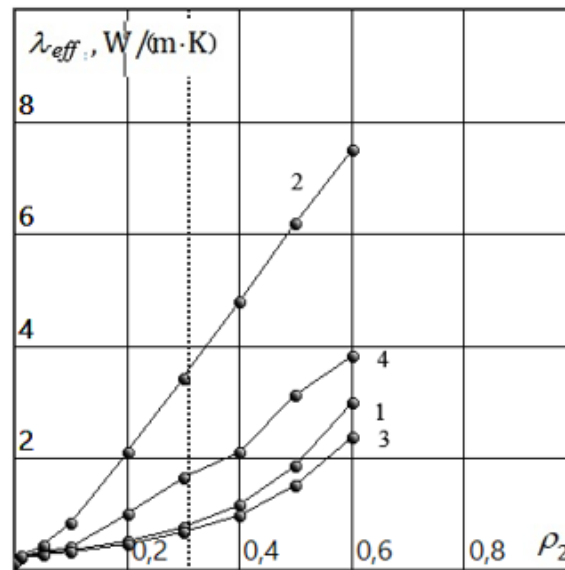


Figure 9 – Effective thermal conductivity (ETC) for polyethylene–silicon carbide structures with various orientations: (1) randomly oriented, (2) longitudinal, (3) transverse, and (4) fractal.

4. FACTORS

4.1. Matrix modification

We can increase the thermal conductivity of a matrix by raising its degree of crystallinity. When adding a modifier to the matrix, we assume for preliminary evaluation that the entire interfacial region becomes crystalline. Under this assumption, any increase in the overall degree of crystallinity depends on two factors: the particle–matrix contact area and the thickness of the interfacial region. Fig. 9 presents these relationships. Fig. 10-1 plots the contact area between the particles and the matrix, as well as the clustering coefficient. Fig. 10-2 shows that the degree of crystallinity rises with longer filler concentrations. As we can see, within standard operating concentrations, the filler only causes a very small increase in crystallinity at the interfacial layer.

4.2. Size effects

On the one hand, decreasing the filler particle size increases the interfacial surface area at any given concentration. This increases the relative proportion of crystallites in the matrix due to inoculation compared to the amorphous fraction, which generally raises the effective thermal conductivity of the matrix. On the other hand, a smaller particle size can reduce thermal conductivity due to phonon scattering at particle boundaries. Fig. 11 presents experimental dependencies [3] of the effective thermal conductivity, which clearly demonstrate the influence of this dimensional factor.

Paper [14] discusses how thermal conductivity depends on the size factor and examines energy transfer mechanisms in nanosystems. Furthermore, paper [15] explains the influence of particle size on the thermal conductivity coefficient. This effect occurs due to shifting energy transfer mechanisms in small particles, namely diffusion and ballistic transport [16].

$$\lambda_{eff} = \frac{1}{3} \sum_i \int k_B (\hbar \omega_i / (k_B T))^2 \frac{\exp(\hbar \omega_i / (k_B T))}{\exp \hbar \omega_i / (k_B T) - 1} v_i(k) l_i(k) \cos^2 \Theta dk, \quad (36)$$

where:

k_B – Boltzmann constant; k – the angular deviation between the wave vector and the energy flow; ω_i

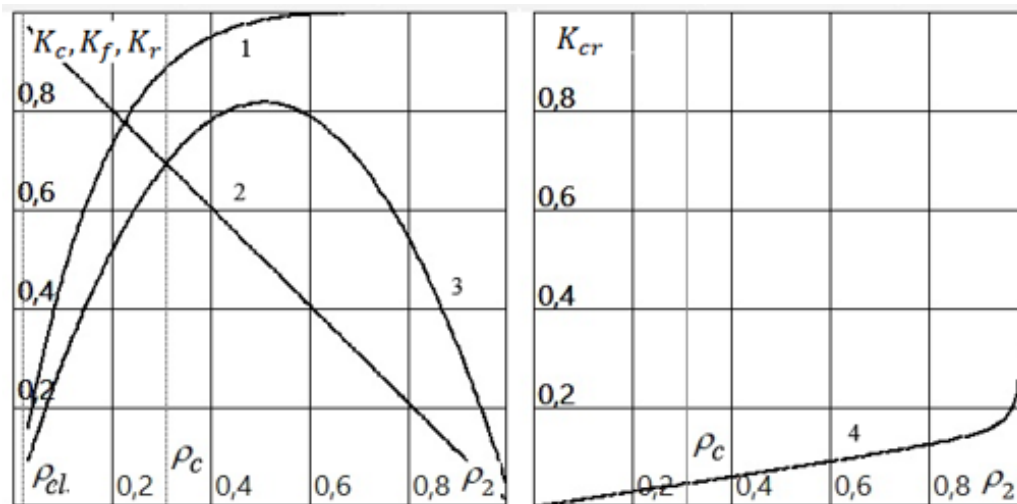


Figure 10 – Clustering coefficients

1. $K_c = N_c/N$ – Clustering coefficient; 2. $K_f = F_m/F_f$ – contact ratio; 3. $K_r = F_m/F_c$ – particle–matrix contact coefficient; 4. $K_{cr} = V_{cr}/V$ – degree of crystallinity; F_f – Total surface area of particles; F_c – Particle–matrix contact area at the percolation threshold; N_c – Number of particles in clusters; N – Total number of filler particles; ρ_c – Percolation threshold; ρ_{cl} – Clustering threshold, the critical concentration for the onset of clustering; V_{cr} – Volume of the crystalline phase of the polymer; V – Total polymer volume.

– the frequency, v_i – group velocity, τ_i – phonon relaxation time, $\hbar$ – Planck-Dirac constant.

Usually, the nanoscale range is defined as up to 100 nm. However, this threshold varies by substance. The unique physical properties of a material appear when the number of internal atoms is roughly equal to the number of surface atoms. Additionally, for dielectrics and semiconductors, the phonon mean free path (the average distance a particle travels before it collides) is a key factor. Therefore, we can use this distance as the maximum limit of nanoscale size for these materials.

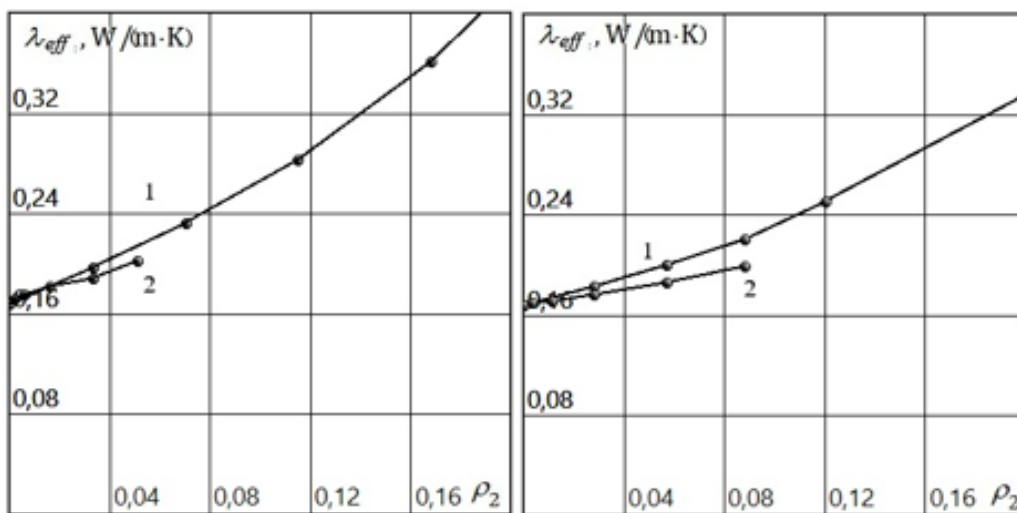


Figure 11 – Experimental dependencies of effective thermal conductivity (ETC) on filler particle size, 1) Epoxy resin + Al_2O_3 at particle sizes: $4\ \mu\text{m}$ (1) and $30\ \text{nm}$ (2); 2) Epoxy resin + SiO_2 at particle sizes of $20\ \mu\text{m}$ (1) and $20\ \text{nm}$ (2).

Heat transfer occurs via two primary mechanisms: diffusive and ballistic. These regimes depend on the Knudsen number. Furthermore, the particle-size-dependent thermal conductivity can be

expressed by a simple formula [14]:

$$\lambda_s = \frac{\lambda_0}{1 + Kn}, \quad Kn = \frac{l}{a}; \quad (37)$$

By substituting the phonon mean free path values into equation (1) and varying the particle size, we can determine how the material's thermal conductivity depends on particle dimensions (see Fig. 11).

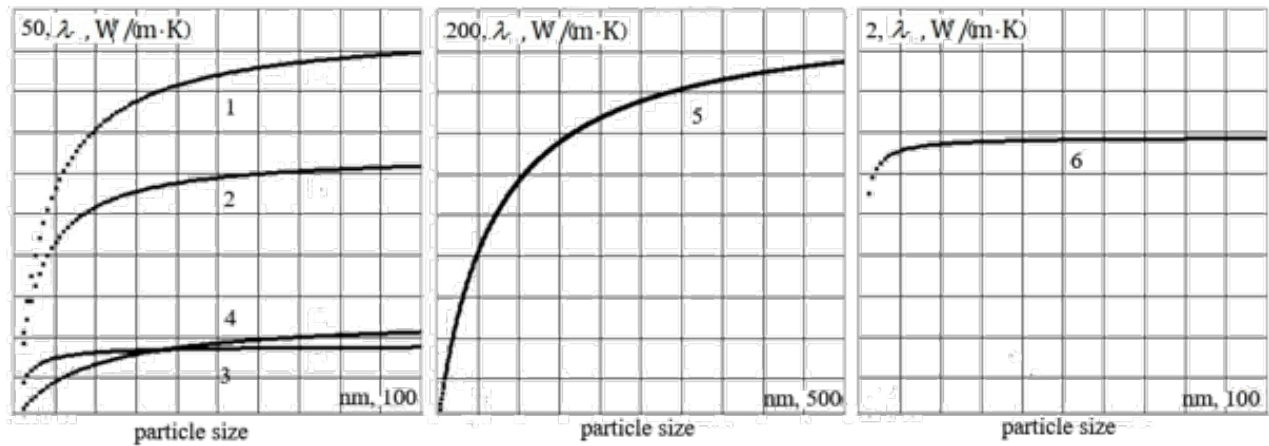


Figure 12 – Dependence of the effective thermal conductivity (ETC) of a particle on its size: 1 – MgO; 2 – Al₂O₃; 3 – TiO₂; 4 – ZnO; 5 – SiC; 6 – SiO₂.

Fig. 12 illustrates that the maximum limit of the nanoscale range, beyond which thermal conductivity remains constant, differs among substances. Furthermore, a reduction in the effective thermal conductivity of the composite relates to an increase in particle-matrix interfacial contacts.

4.3. Interfacial Region

It is well established that a thermal resistance (Kapitza resistance) occurs at the interface of two dissimilar materials, even when the solids are in perfect contact [17]:

Thermal resistance between phases is determined by the interfacial structure and the physicochemical interaction (adhesion) between the matrix and the filler. At the same time, there are practically no simple formulas to determine the thickness of the interfacial layer [18]:

$$\delta_f = \lambda_1 \frac{D_c}{2} \left\{ 1 - \rho_{fp}^{-1/3} \left[\frac{1}{11} \left(\frac{E_c}{E_1} - 1 \right) \right]^{1/1.7} \right\} \quad (38)$$

E_c, E_1 – the modulus of elasticity of the composite and the matrix, respectively;

ρ_{fp} – unaggregated filler volume fraction.

The application of these formulas is limited by the need to know several parameters that are difficult to determine experimentally (e.g., polymer-particle interfacial tension and polymer melt viscosity).

In [19], the interfacial thermal resistance of finely dispersed fillers is combined with the intrinsic thermal resistance of the particles. Consequently, the thermal conductivity coefficient of the filler, λ_n , is replaced by an effective thermal conductivity coefficient, λ_{neff} .

$$\lambda_{neff} = \frac{\lambda_n}{1 + \frac{R_{K1n}}{d_n}} \quad (39)$$

d_n – mean filler particle size,

By adjusting the thermal interfacial resistance, we achieved alignment between the theoretical and experimental curves. Experimental data indicates that a composite with an Al_2O_3 filler concentration of 0.312 exhibits an effective thermal conductivity (ETC) of $0.675 \text{ W}/(\text{m} \cdot \text{K})$. Because direct experimental methods to determine Kapitza thermal layer parameters—such as thermal resistance and thickness—are currently unavailable, we evaluated combined analytical and numerical approach. One such variant is detailed in. Given reliable experimental ETC data for a composite, numerical simulations can be performed using the Kapitza layer's thermal resistance as a fitting parameter. When the experimental and calculated ETC values match, the thickness of the Kapitza thermal layer is determined using its thermal resistance and effective thermal conductivity. In this study, optimal convergence was achieved at a thermal resistance of $10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$, yielding a Kapitza layer thickness of 6.75 nm. This value is consistent with the literature, where reported thermal interfacial layer thicknesses range from 1 to 22 nm.

Research [20] explores methods to determine the effective thermal conductivity (ETC) of epoxy composites filled with carbon nanotubes. These studies confirm that adding a highly thermally conductive filler does not guarantee a high overall ETC for the composite. The main challenge is the poor thermal transfer between filler particles. This issue occurs because of interfacial thermal resistance and contact resistance between the nanotubes. The thermal contact resistance for overlapping nanotubes is $6.46 \cdot 10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$ across a 2.5 nm distance. Other simulations estimate this value at $8.3 \cdot 10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$. These values were found for nanotubes that are 6 nm in diameter and 8 nm to 40 nm in length. Additionally, thermal resistance increases sharply when the gap between fibers exceeds 10 Å. Reference [21] further explains why highly conductive composites are difficult to achieve, even with carbon nanotube fillers. Finally, research [22] shows that thermal resistance is higher when nanotubes are arranged longitudinally (end-to-end) compared to a transverse (side-by-side) fiber arrangement.

The assessment of the interfacial thermal resistance can be made according to the acoustic mismatch model [23]:

$$R_c = \frac{2(\rho_1 v_1 + \rho_2 v_2)^2}{C_1 \rho_1^2 v_1^2 \rho_2 v_2} \left(\frac{v_2}{v_1} \right)^2 \quad (40)$$

Equation (40) yields interfacial thermal resistance values on the order of 10^{-8} for the composites considered above $10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$.

5. CONCLUSIONS

Preliminary calculations of the effective thermal conductivity (ETC) in composites significantly reduce the labor required to develop materials with specific physical properties. However, classical empirical models struggle to adapt to unique compositional systems, particularly at filler concentrations below 0.1%. Numerical methods offer the most successful approach, as they can account for a wide variety of variables. Consequently, increasing the ETC of polymer-based composites for electronic heat dissipation depends on multiple design factors (Table 1).

Although the high thermal conductivity of fillers increases the effective thermal conductivity (ETC) of polymer composites, this effect is only significant at concentrations above the percolation threshold (0.311). Unlike the sharp increase observed in electrical hopping conductivity, experimental and numerical evaluations of the effective thermal conductivity show no such jump. This is because contact thermal resistance increases as particle clusters grow. According to the tabulated data, the filler's intrinsic thermal conductivity mainly plays a role at relatively high values. While filler particles alter the boundary layer by increasing its thermal conductivity, the total volume of this

Table 1. Factors Affecting the Effective Thermal Conductivity of a CS.

Factor	$\rho_2 = 0.5\%$	$\rho_2 = 20\%$	$\rho_2 = 60\%$
Thermal conductivity of the matrix	+	+	—
Thermal conductivity of the filler	—	+	+
Modification	+	—	—
Filler agglomerates	—	+	+
Interfacial Contact		+	—
Contact resistance of filler particles	—	+	+
Size effects		+	+

interfacial space is too small to significantly affect the overall ETC. Furthermore, the Kapitza thermal resistance—the temperature drops at the interface between the filler and the matrix—acts as a barrier. Together with the thermal resistance between the particles within the cluster, this resistance prevents a major increase in composite ETC, even when highly conductive fillers (like carbon nanotubes) are used.

The following factors exert a decisive impact on the effective thermal conductivity of the composite and warrant further investigation: the manufacturing technique of the composite, the clustering and percolation structuring of the filler within the matrix, and the interfacial thermal contact resistance between the filler particles.

At low filler concentrations (until clusters are formed), the effective thermal conductivity is completely determined by the properties of the matrix. In fact, at low concentrations, the ratio of the effective thermal conductivity to the thermal conductivity of the matrix $K = \lambda_{eff}/\lambda_1$ is a characteristic of the modifier. The concentrations of the filler at which the factors affecting the effective thermal conductivity (thermal conductivity of the matrix, thermal conductivity of the filler, inoculation, clustering of the filler, interfacial resistance, contact resistance of filler particles) are significant.

At low filler concentrations—before filler clusters or continuous networks form—the effective thermal conductivity is determined entirely by the properties of the matrix. In fact, the ratio of the effective thermal conductivity to the matrix's thermal conductivity $K = \lambda_{eff}/\lambda_1$ serves as a primary characteristic of the modifier at these low concentrations. However, as filler concentration increases, several additional factors become significant in determining the effective thermal conductivity.

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