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Calculation of the effective thermal properties of the composites based on the finite element solutions of the boundary value problems

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Abstract. One of the key problems of mechanics of composite materials is an estimation of effective properties of composite materials. This article describes the algorithms for numerical evaluation of the effective thermal conductivity and thermal expansion of composites. An algorithm of effective thermal conductivity evaluation is based on sequential solution of boundary problems of thermal conductivity with different boundary conditions (in the form of the temperature on the boundary) on representative volume element (RVE) of composite with subsequent averaging of the resulting vector field of heat flux. An algorithm of effective thermal expansion evaluation is based on the solution of the boundary problem of elasticity (considering the thermal expansion) on a RVE of composite material with subsequent averaging of a resulting strain tensor field. Numerical calculations were performed with the help of Fidesys Composite software module of CAE Fidesys using the finite element method. The article presents the results of numerical calculations of the effective coefficients of thermal conductivity and thermoelasticity for two types of composites (single-layer fiber and particulate materials) in comparison with the analytical estimates. The comparison leads to the conclusion about the correctness of algorithms and program developed.

1. Introduction

At present, in many areas of technology various composite materials (composites) are widely used - artificially created heterogeneous solid materials consisting of two or more components with a clear boundary between them. The composites feature high strength and stiffness combined with lightness and resistance to mechanical, thermal and chemical influence. When combining several components of the composite a material is formed with a set of characteristics that reflect not only the properties of the components, but sometimes some new properties which the components do not possess individually.

When working with composite materials, there is a problem of averaging of their mechanical or physical properties. With the known geometry of the composite and the known properties of the components it is necessary to calculate the effective (i.e. averaged) properties of the composite material [1, 2, 3]. There are different solutions of this problem - both analytic, using formulas, and numerical, using modern computational tools.


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This article discusses the method of numerical evaluation of effective thermal properties of composites based on the numerical solution of boundary problems on a representative volume element (RVE) of composite material. Calculations on a RVE were performed using the finite element analysis method [4, 5] with the help of CAE Fidesys [6].

2. Method of the effective properties calculating

Since we are talking about calculations on a RVE, one should give a definition of this concept first. The representative volume element (RVE) of composite material is the minimal volume of the material, which can be used for some experiments and measurements, on the basis of which it is possible to draw conclusions about the behavior of the material as a whole. If the composite material features an irregular structure, its RVE should contain a sufficient volume of each component to in order to havbe a possibility to average the properties of the entire material. if a composite features a periodic structure - then a cell of periodicity is an RVE.

2.1. Estimation of effective coefficients of thermal conductivity

We begin with the definition of the effective thermal conductivity. Let's call the homogeneous material**as the effective (averaged) material** (from the point of view of thermal conductivity), if it meets the following condition: if we consider a RVE of the initial composite material and fill the exact same volume of with this homogeneous material, then the average (averaged by volume) vectors of the heat flow in these two volumes will be equal at the same temperatures at the boundaries of the volumes. Let's call the thermal conductivity of this material as the **effective thermal conductivity**.

Let's describe a methodology for estimation of the effective thermal conductivity of the composite material using this definition. For a RVE V in the form of a rectangular parallelepiped sized $2A$x$2B$x$2C$ we will solve a certain number of boundary problems of thermal conductivity [7] (for steady thermal state with no internal heat sources):

$$\nabla \cdot q = 0 \tag{1}$$

with *nonperiodic* boundary conditions in a form of predetermined temperature on the boundary

$$T\big|_{\Gamma} = \nabla T^e \cdot r \tag{2}$$

or with *periodic* boundary conditions in the form of bonds to temperatures of corresponding to each other points on the opposite faces of a RVE

$$\begin{aligned} T_i - T_{-i} &= 2A \cdot (\nabla T^e)_1 \\ T_j - T_{-j} &= 2B \cdot (\nabla T^e)_2 \\ T_k - T_{-k} &= 2C \cdot (\nabla T^e)_3 \end{aligned} \tag{3}$$

where ∇ is gradient operator, q is heat flux vector, T is temperature, r is radius vector of a point on the boundary. For *periodic* boundary conditions (i, $-i$), (j, $-j$), (k, $-k$) are pairs of points corresponding to each other on opposite sides of the RVE.

Here ∇T^e is a kind of effective temperature gradient on a RVE, which we are setting up. Each boundary thermal conductivity problem corresponds to separate effective temperature gradient. For *periodic* boundary conditions $(\nabla T^e)_1, (\nabla T^e)_2$, $(\nabla T^e)_3$ are components of the gradient.

As a result of each task solution, we will get a vector distribution of the heat flux q over the RVE. Let's average it by the volume according to the formula

$$q^e = \frac{1}{V}\int_V q dV \tag{4}$$

and we will obtain an efficient vector of heat flux q_e. The effective thermal conductivity of the composite will be evaluated in the form of relation of q_e, obtained by us as a result of the calculation, to the effective temperature gradient ∇T^e, which we have defined as an input - in a form of Fourier law for thermal conductivity:

$$q_i^e = -\lambda_{ij}\left(\nabla T^e\right)_j \tag{5}$$

In order to calculate the effective thermal conductivity coefficients, which we are interested in, we will solve three boundary thermal conductivity problems corresponding to the following temperature gradients:

1) $\nabla T^e = (\delta;0;0) \Rightarrow \lambda_{i1} = -\dfrac{q_i^e}{\delta}, i = 1,2,3$

2) $\nabla T^e = (0;\delta;0) \Rightarrow \lambda_{i2} = -\dfrac{q_i^e}{\delta}, i = 1,2,3$

3) $\nabla T^e = (0;0;\delta) \Rightarrow \lambda_{i3} = -\dfrac{q_i^e}{\delta}, i = 1,2,3$

Thus, by solving these three problems, we calculate all the effective thermal conductivity coefficients of the composite material.

2.2. Estimation of the effective coefficients of thermal expansion

First, let's define the effective thermal expansion. Let's call the effective (as averaging) material (in terms of thermal expansion) such a homogeneous material which meets the following condition: if we consider a RVE of the initial composite material and fill the exact same volume with this homogeneous material, then the average (averaged by volume) thermal strain of these volumes will be equal at the same temperature distribution over the volumes. The coefficients of thermal expansion of the material will be called as effective coefficients of thermal expansion.

Let's describe a methodology for estimation of the effective thermal conductivity of the composite material using this definition. For a RVE V_0 in the form of a rectangular parallelepiped sized $2A$x$2B$x$2C$ wewill solve a certain number of elastic boundary value problems [8] considering the thermal expansion:

$$\begin{aligned} \nabla \cdot \sigma^{el} &= 0 \\ \sigma^{el} &= \sigma - \sigma^{th} \end{aligned} \tag{6}$$

In (6) σ is total stress tensor, σ^{el} is mechanic (elastic) stress tensor, σ^{th} is thermal stress tensor.

At the same time *nonperiodic* or *periodic* boundary conditions are applied to the RVE, and the entire volume is heated to ΔT. Under the influence of temperature the volume deforms (freely expands). By averaging the strain tensor over the volume (in the final state after deformation) we will obtain an effective strain tensor:

$$\varepsilon^e = \frac{1}{V}\int_V \varepsilon dV \tag{7}$$

Let's find the effective thermal expansion

$$\varepsilon_{ij}^{th} = \alpha_{ij}\Delta T \tag{8}$$

where ε^{th} is thermal strains tensor. A value of ΔT, to which a RVE was heated, was set up by us; and the effective strain tensor resulting from this heating was calculated. Effective thermal expansion coefficients are calculated according to the formula:

$$\alpha_{ij} = \frac{\varepsilon_{ij}^{e}}{\Delta T} \tag{9}$$

Boundary conditions applied to the RVE, should be discussed separately. *Nonperiodic* boundary conditions in this problem are zero pressure on the border of the volume, which allows it to expand freely as the temperature increases. *Periodic* boundary conditions also allow the volume to expand freely, with only one restriction: the RVE which was the periodicitycell prior to the deformation of the composite, should remain to be the periodicity cell after deformation.

For this purpose a pair of points (1, 2) is fixed, the first point lies on the edge $x = A$, the second point lies on the edge $x = -A$, and their projections match each other (these could be the corner points). And for the displacement of each pair of points (i, $-i$), the first of which lies on the edge $x = A$, the second one lies on the edge $x = -A$ a relationship is put on:

$$\vec{u}_1 - \vec{u}_2 = \vec{u}_i - \vec{u}_{-i} \tag{10}$$

where u is the displacement vector of a point. Once again, we note that pairs of points (i, $-i$) in (10) are varied, passing across the surface of edges $x = A$ and $x = -A$; and a pair of points (1, 2) - is a fixed one and the same for all relationships (10).

Relationships similar to (10) are put on points of edges $y = B$ and $y = -B$ and edges $z = C$ and $z = -C$. These boundary conditions allow the model to change its volume freely while remaining the periodicity cell of the composite material by the form.

3. Examples of calculations

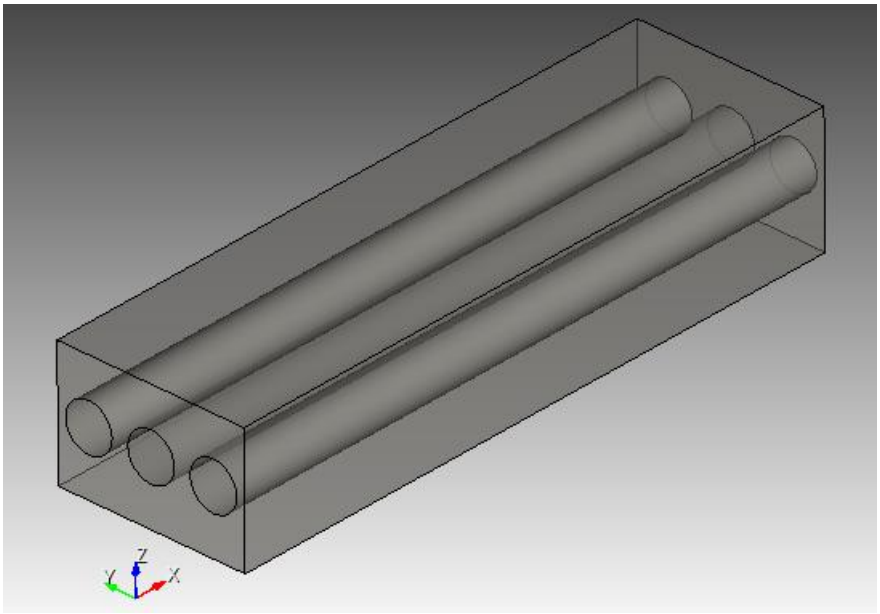
The described methods of numerical evaluation of the effective thermal conductivity and thermal expansion coefficients are implemented in a Fidesys Composite software module of CAE Fidesys. Boundary problems of elasticity and thermal conductivity are solved with the help of computational kernels CAE Fidesys using the finite element analysis method. For example, let's give the numerical solution of the problem of effective evaluation of thermal conductivity and thermal elasticity coefficients for the two types of composites as compared with analytical solutions.

3.1. Single-layer fiber composite

A single-layer fiber composite material is a two component composite material, wherein each layer of matrix is reinforced by unidirectional continuous fibers of the same thickness and the same spacing (Fig. 1). Effective *thermal conductivity* coefficients of such composite material can be estimated using the analytical formulas [9] (in which it is assumed that the fibers are directed along the axis X):

$$\begin{aligned} \lambda_x &= \lambda_f \gamma_f + \lambda_m \gamma_m \\ \lambda_y &= \lambda_z \approx \lambda_m \frac{1 + \gamma_f + \gamma_m \dfrac{\lambda_m}{\lambda_f}}{\gamma_m + (1 + \gamma_f)\dfrac{\lambda_m}{\lambda_f}} \end{aligned} \tag{11}$$

where λ_f and λ_m are thermal conductivity coefficients of the matrix and fibers, respectively, γ_f and γ_m - volumetric concentration of the fibers and the matrix, respectively.



Fiqure 1. Single-layer fiber composite material

Effective *coefficients of thermal expansion* for such composite material can be estimated using formulas [9]:

$$\alpha_x = \frac{\alpha_m E_m \gamma_m + \alpha_f E_f \gamma_f}{E_m \gamma_m + E_f \gamma_f}$$

$$\alpha_y = \alpha_z = \frac{\alpha_f + 2\alpha_m - 2\nu_f \dfrac{\alpha_m - \alpha_f}{1 + \dfrac{E_f \gamma_f}{E_m \gamma_m}} + 2\nu_m s \dfrac{\alpha_m - \alpha_f}{1 + \dfrac{E_m \gamma_m}{E_f \gamma_f}}}{1 + 2s} \tag{12}$$

where $s = 2\left(t_f / d - 1\right)$.

In the formula (12) α_f and α_m are coefficients of thermal expansion of the fibers and the matrix, respectively, γ_f and γ_m are volumetric concentration of the fibers and the matrix, respectively, E_f and E_m are Young's modulus fibers and the matrix, respectively; ν_f and ν_m are Poisson's ratios of the fibers and the matrix, respectively; d is fiber diameter, t_f is fibers spacing (distance between adjacent fibers).

A single-layer fiber composite material with fibers concentration of 10% was considered. Fiber properties: Young's modulus of 2,000 MPa, Poisson's ratio of 0.2, the thermal expansion coefficient of 0.1 K^{-1}, the thermal conductivity of 10 W/(m·K). Matrix properties: Young's modulus of 2 MPa, the Poisson's ratio of 0.3, the thermal expansion coefficient of 0.001 K^{-1}, thermal conductivity coefficient of 2 W/(m·K). Analytical and numerical values of thermal conductivity are listed in Table 1.

Table 1. Coefficients of thermal conductivity of single-layer fiber composite material.

	Analytical, W/(m·K)	Numerical, W/(m·K)
λ_x	2.8	2.78952
λ_y	2.28571	2.27496
λ_z	2.28571	2.27484

Analytical and numerical values of the thermal expansion coefficients are listed in Table 2.

Table 2. Coefficients of thermal expansion of single-layer fiber composite.

	Analytical, K^{-1}	Numerical, K^{-1}
α_x	0.099117	0.099097
α_y	0.005296	0.005087
α_z	0.005296	0.005086

As one can see in the Table 1, the thermal conductivity coefficients for the fiber composite obtained numerically are equal to analytical values with very good accuracy (the error is less than 1%). Table 2 shows that the numerical values of the coefficients of thermal expansion match the analytical with error of not more than 4%, which is also a good accuracy.

3.2. The particulate composite reinforced by spherical inclusions

The particulate composite is a matrix reinforced by individual filler particles. For simplicity, let's consider the numerical calculation model of such a composite in which the filler particles have the same spherical shape, the same size and are arranged in a periodic manner in the martix, and the bulk concentration of filler in the composite is small. Effective *coefficient of thermal conductivity* of such composite can be estimated by the analytical formula [9]:

$$\lambda = \lambda_m \frac{1-2k\gamma_i}{1+k\gamma_i}, \text{ where } k = \frac{\lambda_m - \lambda_i}{2\lambda_m + \lambda_i} \tag{13}$$

where λ_i and λ_m are thermal conductivity coefficient of filler inclusions and the the matrix, respectively, γ_i and γ_m - volumetric concentration of filler inclusions and the matrix, respectively.

Effective *coefficient of thermal expansion* of such composite can be estimated by the formula [9]:

$$\alpha = \overline{\alpha} - \frac{\gamma_m \gamma_i (\alpha_m - \alpha_i)(K_i - K_m)}{\overline{K} + K_i \frac{1+\nu_m}{2(1-2\nu_m)}}, \text{ where } \begin{array}{l} \overline{\alpha} = \alpha_i \gamma_i + \alpha_m \gamma_m \\ \overline{K} = K_i \gamma_i + K_m \gamma_m \end{array} \tag{14}$$

In the formula (14) α_i and α_m are coefficients of thermal expansion of inclusions and the matrix, respectively; γ_i and γ_m are volumetric concentration of inclusions and the matrix, respectively; K_i and K_m are volumetric compression modules of inclusions and the matrix, respectively; ν_i and ν_m are Poisson's ratios of inclusions and the matrix, respectively.

A particulate composite with concentration of spherical inclusions of 5% was considered. Fiber properties: Young's modulus of 10 MPa, Poisson's ratio of 0.25, the thermal expansion coefficient of 0.1 K^{-1}, thermal conductivity coefficient of 10 W/(m·K). Matrix properties: Young's modulus of 1 MPa, the Poisson's ratio of 0.4, the thermal expansion coefficient of 0.001 K^{-1}, thermal conductivity coefficient of 2 W/(m·K). Analytical and numerical values of the thermal conductivity coefficient are shown in Table 3.

Table 3. Coefficient of thermal conductivity of particulate composite material.

	Analytical, W/(m·K)	Numerical, W/(m·K)
λ	2.17642	2.17519

Analytical and numerical values of the thermal expansion coefficient are listed in Table 4.

Table 4. Coefficient of thermal expansion of particulate composite material.

	Analytical, K^{-1}	Numerical, K^{-1}
α	0.006879	0.007077

As one can see in the Table 3, the thermal conductivity coefficient of the particulate composite material obtained numerically match the analytical value with very good accuracy (error is less than 1%). The numerical values of thermal expansion coefficients match the analytical values with the accuracy of no more than 3%, which also shows good accuracy of numerical solution.

4. Conclusion

The article presents the developed algorithm of calculation of effective thermal properties of composite materials on the basis of solving of boundary value problems of thermal conductivity and elastic boundary value problem for a RVE with the subsequent averaging of the results. The algorithm is implemented in a Fidesys Composite software module of CAE Fidesys. The comparison with the known analytical solutions was conducted, which allowed to draw a conclusion about the correctness of algorithms and the program developed. In the future we plan to generalize the approach to the case of nonlinear thermal conductivity and thermo-elasticity models.

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5. References

[1] Levin V A, Zingerman K M, Vershinin A V, Yakovlev M Ya 2015 Numerical analysis of effective mechanical properties of rubber-cord composites under finite strains *Compos. Struct.* **131** pp 25–36.
[2] Vershinin A V, Levin V A, Zingerman K M, Sboychakov A M, Yakovlev M Ya 2015 Software for estimation of second order effective material properties of porous samples with geometrical and physical nonlinearity accounted for *Adv. Eng. Softw.* **86** pp 80–84.
[3] Levin V A, Vdovichenko I I, Vershinin A V, Yakovlev M Ya, Zingerman K M 2016 Numerical estimation of effective mechanical properties for reinforced Plexiglas in the two-dimensional case *Model. Simulat. Eng.* Article ID 9010576 10 pp. Available online: http://www.hindawi.com/journals/mse/2016/9010576/
[4] Zienkiewicz O C, Taylor R L 2000 *The finite element method. Vol. 1. The basis.* (Butterworth-Heinemann: Oxford, United Kingdom) 707 pp.
[5] Zienkiewicz O C, Taylor R L 2000 *The finite element method. Vol. 2. Solid mechanics.* (Butterworth-Heinemann: Oxford, United Kingdom) 479 pp.
[6] Fidesys LLC official website. Available online: http://cae-fidesys.com
[7] Lykov A V 1967 *Theory of Thermal Conductivity* [in Russian] (Moscow: Vysshaya Shkola).
[8] Lurie A I 1990 *Non-Linear Theory of Elasticity* (North-Holland: Amsterdam, Netherlands) 617 pp.
[9] Vishnyakov L R et al. 1985 *Composites* [in Russian] (Kiev: Naukova Dumka) 294 pp.