

PROBABILISTIC EFFECTIVE HEAT CONDUCTIVITY OF FIBER COMPOSITES

Marcin Kamiński

Division of Mechanics of Materials

Technical University of Łódź

Al. Politechniki 6, 93-590 Łódź, POLAND

e-mail: marcin@kmm-lx.p.lodz.pl

Abstract

In the paper an attempt for the probabilistic homogenization in heat conduction problems of fiber composites is presented. On the basis of the effective modules approach applied to scalar fields, numerical method of heat conduction problem homogenization based on the Monte-Carlo simulation (MCS) technique is proposed and implemented in the program MCCEFF. This program has been used to numerical studies of stochastic sensitivity of effective heat conductivity probabilistic moments to different input geometrical as well as material random parameters of the composite being modelled. Computational experiments provided in the paper show probabilistic moments up to fourth order of effective conductivity coefficient as well as its upper and lower bounds. Moreover, the probabilistic convergence of results with increasing number of random trials used in simulation has been studied. Finally, effectiveness of computational algorithm worked out is verified on the example of heat conduction problem in fiber reinforced composite which has been computed by the use of program ABAQUS.

1. Introduction

Main problem with computational analysis of multicomponent (composite) media by the use of different discrete grid or non-grid methods is scale effect occurring in their structure [7]. The problem simplifies when composite considered appears to be periodic what means that there exists some geometrical cell (periodicity cell or representative volume element) which, due to geometric translation, can cover the whole structure. Considering the fact that in most of engineering problems the scale factor relating periodicity cell with whole structure is very small, discretization is very complicated process. To omit this problem, so-called homogenization method is introduced, which allows us to replace original multimaterial composite with equivalent one that can be characterized by homogeneous tensor of material properties. Thus, we can model composite structure

without differentiating the regions belonging to different materials what significantly simplifies meshing procedure [24].

The next engineering problems is how to use experimental data described by mean values and standard deviations of material and physical parameters of the composite constituents to evaluate these effective parameters of the whole composite. Moreover, it is observed that microgeometry in the most of composites have generally random character which can be decisive for their overall macroscopic behaviour. Considering these facts, the homogenization method should be formulated including randomness of composites occurring in different scales in most of constitutive parameters. Some mathematical models have been worked out many years ago [4] however without any numerical implementation. The papers devoted to modern homogenization problems, especially in the context of thermal problems are shown and discussed in [8,21].

The main idea of the paper is to formulate and solve the homogenization problem for heat conduction in two-component fiber-reinforced composites where the conductivity coefficients are random Gaussian variables. The first two probabilistic moments - the expected values and variances of these variables are given. The micro as well as macro geometry of the composite is treated as deterministic. To calculate effective conductivity of the composite the effective modules method is introduced which introduces so-called temperature homogenization function which is periodic on external boundary conditions of the periodicity cell. The natural boundary conditions in the homogenization problem are taken in the form of difference between heat conductivity coefficients of component materials. To compute the expected values, variances and higher order probabilistic moments of effective conductivity, Monte-Carlo simulation technique [10,12] is used consisting of random trials and statistical estimation procedure. This technique has been used widely in another mechanical and physical problems including probabilistic approaches to the homogenization of elasticity tensor presented in [13,14,22]. As it is known [18], there are numerous another mathematical and computational ways to randomize the problems discussed, the stochastic perturbation approach or

expansion by the use of stochastic polynomials [9], however numerical implementations seem to be significantly more difficult than for MCS technique and, moreover, have their well-known limitations on randomness of input random variables [18]. Considering this fact, the homogenization-oriented and FEM-based program MCCEFF has been extended to homogenize the heat conduction problem. Thanks to the numerical algorithm implemented, probabilistic moments up to the fourth order of the effective conductivity coefficient are computed for fiber-reinforced composite. Moreover, the sensitivity of the probabilistic moments with respect to reinforcement ratio, randomness of composite constituents as well as for total number of random trials performed (so-called numerical convergence verification) is verified numerically. Since this fact, that homogenization is only preprocessor to analyze composite materials some heat conduction problem defined on the periodicity cell is solved by using program ABAQUS [1] to verify effectiveness of homogenization procedure.

2. Heat conduction equation

Let us consider a three-dimensional body occupying the region Ω in the steady-state conditions. Let us consider that there is the heat conduction in our body what means that the Ω obeys the Fourier's law:

$$g_x = k_x \frac{\partial \theta}{\partial x}; \quad g_y = k_y \frac{\partial \theta}{\partial y} \quad 1.$$

where g_x and g_y are the heat flows conducted per unit area, θ is the temperature of the body, while k_x , k_y are the thermal conductivities corresponding to the principal axes x , y . Considering the heat flow equilibrium in the interior of the body considered, we have:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial \theta}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial \theta}{\partial y} \right) = g \quad 2.$$

where g is the rate of heat generated per unit area. On the external boundaries of Ω the following conditions are satisfied

$$\theta|_{\partial\Omega_\theta} = \hat{\theta} \text{ and } k_n \frac{\partial\theta}{\partial n}|_{\partial\Omega_q} = \hat{q} \quad 3.$$

where $\hat{\theta}$ is the known surface temperature on boundary $\partial\Omega_\theta$, k_n is the body thermal conductivity, n denotes the coordinate axis in the direction of the unit normal vector \mathbf{n} (pointing outward) to the surface, \hat{q} is the prescribed heat flux input on the surface $\partial\Omega_q$ of the body and

$$\partial\Omega_\theta \cup \partial\Omega_q = \partial\Omega \text{ and } \partial\Omega_\theta \cap \partial\Omega_q = \{\emptyset\} \quad 4.$$

Introducing the summational convention we have the above equations in the following form

$$\sum_{i=1,2} (k_i \theta_{,i})_{,i} + g = 0 \quad (\text{no sum on } i) \quad 5.$$

$$\theta = \bar{\theta}; \quad x \in \partial\Omega_\theta \quad (\text{essential boundary conditions}) \quad 6.$$

$$k_n \theta_{,n} = \bar{q}; \quad x \in \partial\Omega_q \quad (\text{natural boundary conditions}) \quad 7.$$

To obtain the variational formulation of the problem considered we multiply eqn (5) by virtual temperature distribution $\delta\theta$ and integrate over the whole Ω . We arrive at

$$\left(\sum_{i=1,2} \int_{\Omega} (k_i \theta_{,i})_{,i} d\Omega + \int_{\Omega} g d\Omega \right) \delta\theta = 0 \quad 8.$$

It should be underlined that arbitrary character of $\delta\theta$ causes that formulations (5) and (8) are to be equivalent. Further, observing that

$$[\delta\theta (k_i \theta_{,i})]_{,i} = \delta\theta_{,i} (k_i \theta_{,i}) + \delta\theta (k_i \theta_{,i})_{,i} \quad 9.$$

and

$$\frac{\partial(\delta\theta)}{\partial x_i} = \delta\theta_{,i} \quad 10.$$

we obtain

$$\sum_{i=1,2} \int_{\Omega} (\delta\theta k_{i,\theta_{,i}})_{,i} d\Omega - \sum_{i=1,2} \int_{\Omega} \delta\theta_{,i} k_{i,\theta_{,i}} d\Omega + \int_{\Omega} g\delta\theta d\Omega = 0 \quad 11.$$

what, neglecting the rate of heat generated g (assuming no coupling between mechanical and thermal effects and steady state conditions) can be rewritten as

$$\sum_{i=1,2} \int_{\Omega} (\delta\theta k_{i,\theta_{,i}})_{,i} d\Omega - \sum_{i=1,2} \int_{\Omega} \delta\theta_{,i} k_{i,\theta_{,i}} d\Omega = 0. \quad 12.$$

Considering the divergence theorem in the form of

$$\sum_{i=1,2} \int_{\Omega} (\delta\theta k_{i,\theta_{,i}})_{,i} d\Omega = \sum_{i=1,2} \int_{\partial\Omega} \delta\theta k_{i,\theta_{,i}} n_i d(\partial\Omega) = \int_{\partial\Omega} \delta\theta k_n \theta_{,n} d(\partial\Omega). \quad 13.$$

we obtain from eqn (12) that

$$\sum_{i=1,2} \int_{\Omega} \delta\theta_{,i} k_{i,\theta_{,i}} d\Omega - \int_{\partial\Omega} \delta\theta k_n \theta_{,n} d(\partial\Omega) = 0. \quad 14.$$

Taking into account the natural boundary condition (7) and the fact that $\delta\theta = 0$ on $\partial\Omega_\theta$ we obtain finally

$$\sum_{i=1,2} \int_{\Omega} \delta\theta_{,i} k_{i,\theta_{,i}} d\Omega = \int_{\partial\Omega_q} \delta\theta \hat{q} d(\partial\Omega). \quad 15.$$

This is the principle of virtual temperatures corresponding to the condition of stationarity of the following functional

$$\pi(\theta) = \frac{1}{2} \sum_{\Omega} \int_{\Omega} k_i(\theta_{,i})^2 d\Omega - \int_{\partial\Omega_q} \theta \hat{q} d(\partial\Omega) \quad 16.$$

what is the basis for finite element formulation of the homogenization problem.

3. Periodic structure model

The main problem presented in the paper is to find the probabilistic distribution of the effective heat conduction coefficient for the whole class of random composite structures which are periodic and made of two components. For this purpose let us assume that Y is periodic in stochastic sense if for an additional ω belonging to a suitable probability space there exists such a translation of Ω which covers the whole region occupied by Y . Since the translation is assumed to be ergodic, thus the ensemble averaging is equivalent to the spatial one. Next, we assume that the section $Y \subset \mathbb{R}^2$ of this composite with $x_3 = 0$ plane is constant along the x_3 axis. The section of the composite considered in the direction orthogonal to the parallel fibers has been shown in Fig. 1.

Let further region Ω contains two perfectly bonded, coherent and disjoint subsets Ω_1 (fiber) and Ω_2 (matrix) and let the scale between respective geometrical diameters of Ω and Y is described by the small parameter $\varepsilon > 0$. Let $\partial\Omega$ denotes external boundary of the Ω while $\partial\Omega_{12}$ - the interface boundary between Ω_1 and Ω_2 regions. Moreover, let Ω_1 and Ω_2 contain transversely isotropic materials for which the heat conduction coefficients are cut-off Gaussian random variables defined as follows

$$0 < k(x; \omega) < \infty \quad 17.$$

$$E[k(x; \omega)] = \begin{cases} k_1; & x \in \Omega_1 \\ k_2; & x \in \Omega_2 \end{cases} \quad 18.$$

$$\text{Cov}(k_i(x; \omega), k_j(x; \omega)) = \begin{bmatrix} \text{Var } k_1 & 0 \\ 0 & \text{Var } k_2 \end{bmatrix} \quad 19.$$

Zeroing of the respective terms of covariance matrix follows the lack of experimental data describing probabilistic correlation of heat conductivities

in fiber and matrix. In the context of definitions (17-19) the periodicity of the composite structure is equivalent to periodicity of probability density functions (PDFs) heat conductivity coefficient (or any either physical or material property). Moreover, taking into account assumption of Gaussian character of these variables, we obtain as effect periodicity in first two probabilistic moments of coefficient under considerations. It may be proved that the periodicity in the context of expected values and variances is not sensitive to PDFs cutting-off.

4. Homogenization problem formulation

The main purpose of the homogenization procedure is to find the effective conductivity coefficient $k^{(eff)}$ characterizing the whole composite and for which an energy defined by eqn (16) is equal to this obtained for the composite in primary configuration. To derive $k^{(eff)}$ the following algorithm is provided:

1. indicating of the Representative Volume Element (RVE) of the composite structure which has minimal geometric dimensions and due to some translation can cover the whole space occupied by composite structure considered. The external shape of the RVE is usually introduced as rectangle or honeycomb (for 2D analysis) or cube (for 3D case).
2. assuming that the essential and natural boundary conditions on $\partial\Omega$ are to be periodic, i.e. temperatures are equal on opposite boundaries of periodicity cell
3. introducing the homogenization function Φ which is in fact some special temperature field and which fulfills the periodicity conditions (values are equal on the opposite sides of periodicity cell).

Thus, we can rewrite variational formulation (13) for the two-component composite as follows

$$\begin{aligned} & \sum_{i=1,2} \int_{\Omega_i} (\delta\theta k_i^{(1)} \theta_{,i})_{,i} d\Omega + \int_{\Omega_2} (\delta\theta k_i^{(2)} \theta_{,i})_{,i} d\Omega + \\ & - \int_{\partial\Omega_1} \delta\theta k_n^{(1)} \theta_{,n} d(\partial\Omega) + \int_{\partial\Omega_2} \delta\theta k_n^{(2)} \theta_{,n} d(\partial\Omega) = 0 \end{aligned} \quad 20.$$

Since the components of the composite are perfectly bonded $\partial\Omega_{12} = \partial\Omega_1 = \partial\Omega_2$ is an interface and we obtain

$$\sum_{i=1,2} \int_{\Omega_i} (\delta\theta k_i^{(1)} \theta_{,i})_{,i} d\Omega + \int_{\Omega_2} (\delta\theta k_i^{(2)} \theta_{,i})_{,i} d\Omega - \int_{\partial\Omega_{12}} \delta\theta (k_n^{(1)} - k_n^{(2)}) \theta_{,n} d(\partial\Omega) = 0. \quad 21.$$

which due to the divergence theorem given by eqn (13) can be rewritten as

$$\sum_{i=1,2} \left(\int_{\Omega_i} (\delta\theta k_i^{(1)} \theta_{,i})_{,i} d\Omega + \int_{\Omega_2} (\delta\theta k_i^{(2)} \theta_{,i})_{,i} d\Omega \right) = \sum_{i=1,2} \int_{\partial\Omega_{12}} \delta\theta [k_i] \theta_{,i} n_i d(\partial\Omega). \quad 22.$$

where $[k]$ denotes the respective difference of heat conductivities on the interface $\partial\Omega_{12}$.

Next, let us note that the homogenization function Φ is so defined that the eqn (22) takes the form [6,25]

$$\int_{\Omega_1} [\delta\theta (k_i^{(1)} \Phi_{,i})]_{,i} d\Omega + \int_{\Omega_2} [\delta\theta (k_i^{(2)} \Phi_{,i})]_{,i} d\Omega = \int_{\partial\Omega_{12}} \delta\theta [k_i] n_i d(\partial\Omega). \quad 23.$$

This result follows limiting transition of variational statement of equilibrium equations for real composite with $\varepsilon \rightarrow 0$ [23] what is equivalent to decreasing of geometrical dimensions of periodicity cell.

To compute the effective conductivity let us notice that the LHS of the equation (23) can be jointed to represent an integral over the whole set Ω . To transform the RHS, let us observe that, considering equation (9) we have

$$\begin{aligned} \int_{\Omega} (\delta\theta k_i)_{,i} d\Omega &= \int_{\Omega} \delta\theta_{,i} k_i d\Omega + \int_{\Omega} \delta\theta k_{i,i} d\Omega = \\ &= \int_{\partial\Omega} k_i n_i \delta\theta d(\partial\Omega) - \int_{\partial\Omega_{12}} [k_i] n_i \delta\theta d(\partial\Omega) + \int_{\Omega} \delta\theta k_{i,i} d\Omega \end{aligned} \quad 24.$$

Further

$$\int_{\partial\Omega} k_i n_i \delta\theta d(\partial\Omega) = 0 \quad 25.$$

what follows periodicity condition on $\partial\Omega$, and next

$$\int_{\Omega} \delta\theta k_{i,i} d(\partial\Omega) = 0 \quad 26.$$

what is the result of constant character of the conductivity coefficient k .

Thus we arrive at:

$$\int_{\Omega} (\delta\theta k_i)_{,i} d\Omega = \int_{\partial\Omega_2} [k_i] n_i \delta\theta d(\partial\Omega) \quad 27.$$

what included into the eqn (23) gives

$$\sum_{i=1,2} \left(\int_{\Omega} [\delta\theta (k_i \Phi_{,i})]_{,i} d\Omega \right) = \int_{\Omega} [\delta\theta k_i]_{,i} d\Omega. \quad 28.$$

Thus, the effective conductivity can be calculated as [15]

$$\int_{\Omega} k_i^{(eff)} d\Omega = \int_{\Omega} k_i d\Omega - \int_{\Omega} k_i \Phi_{,i} d\Omega \quad 29.$$

and taking into account that $k_i^{(eff)} = \text{const}$ we can derive

$$k_i^{(eff)} = \frac{1}{|\Omega|} \int_{\Omega} k_i d\Omega - \frac{1}{|\Omega|} \int_{\Omega} k_i \Phi_{,i} d\Omega \quad 30.$$

Finally, introducing $k=k_i$, what follows the isotropic nature of the composite constituents in the plane considered, we have

$$k^{(eff)} = \frac{1}{|\Omega|} \sum_{a=1,2} \int_{\Omega_a} k^{(a)} (1 - 1_i \Phi_{,i}) d\Omega \quad 31.$$

where 1_i is the unity matrix. It should be mentioned that all these transformations are well-known from the homogenization of the elasticity tensor components. The detailed mathematical considerations on existence and uniqueness of homogenization function as well as effective conductivity coefficient can be found in [6,25].

Having computed the expected value of effective heat conductivity coefficient we can compare its value with so-called upper and lower bounds in well-known Voigt-Reuss form:

$$\sup k = \frac{\Omega_1 \cdot k_1 + \Omega_2 \cdot k_2}{\Omega}, \quad 32.$$

$$\inf k = \frac{\Omega \cdot k_1 \cdot k_2}{\Omega_1 \cdot k_2 + \Omega_2 \cdot k_1} \quad 33.$$

Starting from equations (32) and (33) we can evaluate probabilistic moments of these quantities by the use of probabilistic simulation technique. Moreover, it can be observed that in the case of randomly defined conductivity coefficients of composite components, the expected values and variances of the upper bounds (as well as any moments of higher order) can be derived by the use of classical probability theory theorems as follows

$$E[\sup k] = \left(\frac{\Omega_1}{\Omega}\right) \cdot E[k_1] + \left(\frac{\Omega_2}{\Omega}\right) \cdot E[k_2] \quad 34.$$

$$\text{Var}(\sup k) = \left(\frac{\Omega_1}{\Omega}\right)^2 \cdot \text{Var}(k_1) + \left(\frac{\Omega_2}{\Omega}\right)^2 \cdot \text{Var}(k_2) \quad 35.$$

5. Finite element implementation

Let us assume that region Ω is discretized by a set of finite elements and the scalar temperature field Φ is described by the nodal temperatures vector Ψ_α as, cf. [19,20]:

$$\Phi(x_i) = H_\alpha(x_i) \Psi_\alpha; i=1,2 \quad 36.$$

where N is the total number of degrees of freedom of the region Ω . It follows that

$$\Phi_{,i} = H_{\alpha,i} \Psi_\alpha \quad 37.$$

The heat conductivity matrix $K_{\alpha\beta}$ and the vector P_α can then be expressed as follows:

$$K_{\alpha\beta} = \int_{\Omega} k_{ij} H_{\alpha,i} H_{\beta,j} d\Omega \quad 38.$$

and

$$P_\alpha = \int_{\Omega} g H_\alpha d\Omega + \int_{\partial\Omega} \hat{q} H_\alpha d\Omega \quad 39.$$

Using equations (38) and (39), the functional (16) can be rewritten in the following form

$$\pi(\Psi_\alpha) = \frac{1}{2} K_{\alpha\beta} \Psi_\alpha \Psi_\beta - P_\alpha \Psi_\alpha \quad 40.$$

The stationarity conditions of $\pi(\Psi_\alpha)$ lead us to the following equations

$$K_{\alpha\beta} \Psi_\beta = P_\alpha \quad 41.$$

Solving this equation for Ψ_β enables to compute discretized values of the homogenization function and, finally, the effective thermal conductivity coefficient given by equation (31). If parameter 'k' is taken as Gaussian random variable and is defined by the expected values vector $E[k]$ and variances vector $\text{Var}(k)$ we may compute the expected values and

variances of the random temperature field in considered region by the use of Monte-Carlo simulation technique described below.

6. Probabilistic approach to homogenization

We shall now find out expected values and variances of the effective conductivity coefficient. To this end we first have to determine the first two probabilistic moments of the homogenization function. It is known that the probabilistic moments of the random temperature field can be computed alternatively by the Monte-Carlo simulation, von Neumann expansion (or its modern modifications), or stochastic perturbation approaches. Using statistical techniques we solve a large set of corresponding deterministic samples with the conductivity coefficients randomly generated [5] in the whole of the probability space.

Defining appropriate estimators [3] of the effective heat conductivity coefficient we obtain first expected value of the effective conductivity coefficient as

$$E[k^{(eff)}] = \frac{1}{M} \sum_{j=1}^M k^{(eff)(j)} = \frac{1}{M} \sum_{j=1}^M \langle k \rangle_{\Omega}^{(j)} - \frac{1}{M} \sum_{j=1}^M \langle k 1_i \Phi_{,j} \rangle_{\Omega}^{(j)} \quad 42.$$

where M is total number of samples, which should be established taking into account efficiency of estimators, $o(10^3)$, for instance. Then, another probabilistic characteristics can be computed as follows

- variance and standard deviation

$$\text{Var}(k^{(eff)}) = \frac{1}{M-1} \sum_{j=1}^M \left(k^{(eff)(j)} - E[k^{(eff)}] \right)^2 \quad 43.$$

$$\sigma(k^{(eff)}) = \sqrt{\text{Var}(k^{(eff)})} \quad 44.$$

- ordinary moment of the n -th order for the

$$m_n(k^{(eff)}) = \frac{1}{M} \sum_{i=1}^M (k_i^{(eff)})^n, \quad 45.$$

- central moment of the n-th order estimator

$$\mu_n(k^{(eff)}) = m_n[k^{(eff)} - m_1(k^{(eff)})], \quad 46.$$

- coefficients of variation, assymetry and concentration

$$\alpha(k^{(eff)}) = \frac{\sigma(k^{(eff)})}{E[k^{(eff)}]} \quad 47.$$

$$\beta(k^{(eff)}) = \frac{\mu_3(k^{(eff)})}{\sigma^3(k^{(eff)})} \quad 48.$$

$$\gamma(k^{(eff)}) = \frac{\mu_4(k^{(eff)})}{\sigma^4(k^{(eff)})} \quad 49.$$

It is essential to underline that, in the contrary to another probabilistic approaches, simulation technique assures existence and uniqueness of the effective conductivity coefficients probabilistic characteristics what follows deterministic results and the nature of the statistical estimation methods. Further, it can be seen that the accuracy of the estimation results depend on the total number of random trials performed denoted in equations posed above by M while do not depend at all on the input random variables coefficients of variance. Finally, it can be underlined that the technique applied is difficult to apply to large scale systems considering an increase of simulation time with increasing total number of degrees of freedom and technical problems caused by data storage.

The flowchart for probabilistic simulation procedure can be presented in the form of the following algorithm, see Fig. 2 for instance.

7. Computational experiments

Homogenization computational experiments have been carried out by the use of the composite-oriented program MCCEFF [14,16]. This program enables computations of the composite materials effective characteristics for linear elasticity and thermal problems. Generally, n -phase composite materials may be homogenized in elasticity problems while at present two-component for heat conduction, however upper and lower bounds for effective tensors can be calculated automatically for all cases. Probabilistic thermal problems can be solved only by the use of simulation method in the contrary to the effective elasticity tensor computational procedure where MCS as well as stochastic perturbation methods can be used. Due to the fact, that the program has its internal automatic mesh generator as well as many important simulation tools, the homogenization of the composite media with randomly defined material properties as well as their geometry will be able in the version of the code.

First, the sensitivity of effective heat conductivity coefficient probabilistic moments are verified with respect to the composite reinforcement ratio. It enables to solve the problem how the volume of reinforcement influences the probabilistic moments of conductivity coefficients.

The results of the computational analyses are shown in Figs. 3-6 presented above in the function of fiber volume ratio marked on the horizontal axes. The first figure (Fig. 3) presents the expected values of effective values and their bounds, next (Fig. 4) shows the standard deviations of these characteristics. Fig. 5 illustrates the third-order central moment in function of the fiber volume while in Fig. 6 the fourth-order central probabilistic moments are presented. Generally, it is visible on all these figures that the moments of effective conductivity upper and lower bounds bound the moments of effective heat conductivity coefficient very well. Taking into account the interrelations between all these probabilistic characteristics, the approximation of the effective composite conductivity moments by the respective values of lower bound can be proposed. It is very important considering the shortening of computations time because lower bounds are obtained by simple proportions simulation while the effective heat

conductivity coefficient must be calculated by FEM solution of some heat conduction boundary value problem. Observing first two figures, it should be noted that expected values and standard deviations of upper bounds change linearly while the changes of first two moments of effective parameter and its lower bounds have quite nonlinear character. Changes in 3th and 4th order probabilistic moments are nonlinear for all effective characteristics but the differences between values of moments increase together with increase an order of probabilistic moment being analyzed and for data collected in Fig. 6 is even more than 10 times between upper and lower bounds for effective conductivity coefficient. Considering these interrelations, lower bounds should be used for approximation of the effective behaviour of the composite when for some reasons it is impossible to compute effective quantities due to the homogenization method introduced.

Next, the sensitivity of probabilistic moments the effective conductivity to components conductivities randomness are verified. It gives us an answer to the question how the conductivity coefficients randomness influences the probabilistic moments of conductivity. Numerical results dealing with this problem are presented in Figs. 7-10 - expected values and coefficient of variance are marked on the vertical axes while the coefficients of variance of input conductivities which are equal one another - on the horizontal axes. Figure 7 presents expected values of upper bounds, next one presents the expected values of lower bounds for the effective conductivity tensor. The expected values of effective conductivity coefficient are presented in Fig. 9 while coefficients of variance of the same property are presented in Fig. 10. Vertical axes of these figures illustrate the respective values of these moments and the horizontal ones - values of the effective conductivity coefficient standard deviations of both composite components ('composite randomness'). Generally, it is visible that increase of composite randomness decreases the expected values of effective characteristics and increases their coefficient of variation. Moreover, it can be noticed that relations discussed have, neglecting some computational errors, general linear form similar to changes in input coefficients of randomness for composite constituents.

Next, convergence of probabilistic moments of effective conductivity coefficients has been verified. The main purpose of these experiments was to establish an optimal number of random trials for probabilistic simulation that moments computed are obtained with relatively small numerical error. The results of analysis have been presented in Figs. 11-16. The respective estimators are marked on the vertical axes of the graphs while the total number of random trials on the horizontal ones.

First, it should be noted that the convergence of the expected values estimators have the same character for upper and lower bounds as well as for effective conductivity coefficient, see Figs. 11, 12 and 13. The value of estimator decreases rapidly from maximum reached for 10 random trials to minimum for about 50 iterations. Next, with inverse tendency, increases to 100 trials and asymptotically converges to stable value for about 10^4 iterations. The character of coefficient of variance convergence presented in Fig. 14 is quite similar to the discussed above, however asymptotic changes are more smoothened than for expected values shown on previous figures. The coefficient of assymetry (which should be equal to 0 for Gaussian deviates) decreases from maximum reached at the 10 iterations to the value equal to 0 for 10^4 samples with any asymptotic fluctuations (observed for effective elasticity tensor components estimators). The fourth order probabilistic characteristics in the form of coefficient of concentration (which should be equal to 3 for Gaussian random variables) converges analogically as first and second order characteristics to 3 for 10^4 random iterations in simulation. It should be noted that however the probabilistic parameters are equal to those characteristic for Gaussian random variables, we cannot identify the character of effective heat conductivity coefficient probability density function as Gaussian.

Finally, let us note that the homogenization procedure is only some kind of preprocessing tool to computational analysis of the composite materials. Considering this fact and having computed expected values of effective conductivity coefficient, the last group of computational tests has been devoted to verification of some heat conductivity problem for fiber

reinforced composite (Fig. 17) where the conductivity coefficients have been taken as follows:

- upper bound of effective conductivity coefficient (see Fig. 18 for results),
- effective conductivity coefficient (Fig. 19, as previously),
- real composite structure (Fig. 20, as previously),
- lower bound of effective conductivity coefficient (Fig. 21, as previously).

These tests worked out by the use of program ABAQUS [1] enable to verify which of temperature fields for different homogenization techniques is the nearest to the field obtained for composite in real configuration. This is important considering the differences between computations of upper and lower bounds and the direct homogenization of the composite.

Figures 18-21 present only a half of the periodicity cell due to the vertical symmetry of resulted field with respect to the horizontal axes provided in the half of cell height. Observing resulting fields it is characteristic that temperatures for different ways homogenized composite have uniform distribution in the periodicity cell while isotherms as well as temperature gradients are concentrated in matrix region. Moreover, it is visible that the maximal temperature obtained on the right edge of the cell for the composite with conductivity coefficient equal to the effective value is the nearest to the solution for composite in its real configuration. The difference in this temperature for real and effective configuration is about 10% of the value examined. Moreover, as it was expected, the minimal edge temperature is obtained for the model with lower bound of heat conductivity while the maximum is reached for upper bound on this parameter. While the difference between lower bound and effective conductivity is smaller than between homogenized parameter and upper one, the temperature field for composite with upper bound on effective coefficient better approximate effective behaviour of the composite than the lower bound.

8. Concluding remarks

1. The formulation presented and discussed above describes a new homogenization method for the two-component composite materials with random thermal conductivity. The proposed model enables one to compute

expected values and variances of the effective conductivity by using Monte Carlo simulation based on the finite element method (FEM). Numerical implementations which seem to be effective and easy to provide appear to be efficient tools in studying stochastic sensitivity of effective conductivity to the probabilistic moments of composite component conductivities. At the same time it should be noted that Monte-Carlo simulation technique, applied in the program MCCEFF used in the paper, can be successfully incorporated in any commercial FEM (ABAQUS, for instance) or another discrete method based packages.

2. Computational experiments performed show that all probabilistic moments of $k^{(\text{eff})}$ are well bounded by the moments of their upper and lower bounds $\sup(k)$ and $\inf(k)$. Moreover, it can be seen that lower bound expected values and variances are quite effective approximation of effective conductivity moments what can be useful in computational modeling of nonperiodic composites. Taking into account simulation-based character of the randomization method, the most recommended number of random trials has been verified as about 10^4 . Considering the fact that homogenization presented is, in fact, equivalent to the solution of some boundary value problem, this conclusion deals as well with any Monte-Carlo simulated heat conduction problems with heat conductivity coefficients treated as random. To have a good comparison with another probabilistic approaches to the homogenization, an approach based on the stochastic finite element method (SFEM) is recommended which has been used to stochastic modelling of transient heat transfer in [11]. We may expect, as for effective elasticity tensor probabilistic moments [17], that the expected values for the probabilistic model will be smaller than those obtained by SFEM approach and the relation for the variances (or coefficients of variances) will have the inverse character.

3. The probabilistic homogenization procedure involved may be applied for seepage, torsion, irrotational and incompressible flow, film lubrication, acoustic vibration as well as for electric conduction, electrostatic field, electromagnetic waves and all field problems with stochastically defined material or physical characteristics. To use the results presented in the paper to probabilistic homogenization of another engineering field problems, the well-known analogies [2] may be used successfully to

transform probabilistic moments computed for heat conductivity coefficient to describe different physical field parameters, cf. seepage permeability, shear modulus, electrostatic permittivity or electric conductivity.

4. Starting from the homogenization procedure proposed, the sensitivity of the $k^{(eff)}$ probabilistic moments to components conductivities expectations interrelation may be verified in further computational tests. Moreover, probabilistic (homogenization-based) reliability of the composite structures with parameter sensitivity studies (probabilistic characteristics of material parameters) may be provided. On the other hand, it is easy to extend the model proposed to that applicable for n-component random composites as well as for multicomponent media with stochastic structural defects in analogy to carried out in [16].

5. Finally, it can be posed that it seems to be intuitively sensible that randomness in geometry should be equivalent in some sense and under some special assumptions to the randomness in material parameters. However, it must be proved mathematically (or verified numerically) how to replace probabilistic moments of reinforcement shape, random coordinates of fiber center in periodicity cell or even random number of fibers in RVE in the context of expectations or variances of material and physical properties. Neglecting this remark, the next step in extension of stochasticity in composite materials and homogenization procedures is to randomize microgeometry of periodicity cell together with heat conductivity coefficient or elasticity tensor components.

Acknowledgements

The support of this work by the State Committee for Scientific Research (KBN) under Grant No. 8T11F 008 12 PO 2 is gratefully acknowledged.

References

- [1] ABAQUS, v. 5.7, *User's Manual*. Hibbitt, Karlsson & Sorensen, Inc., Pawtucket 1997.
- [2] Bathe K.J., *Finite Element Procedures*. Prentice Hall, Englewood Cliffs, 1996.
- [3] Bendat J.S., Piersol A.G., *Random Data: Analysis and Measurement Procedures*. Wiley, 1971.

- [4] Beran M.J., Application of statistical theories for the determination of thermal, electrical and magnetic properties of heterogeneous materials. In: Broutman L.J. et al., eds., *Mechanics of Composite Materials*. Academic Press, 1974.
- [5] Boswell M.T. et al., The Art of Computer Generation of Random Variables. In: C.R. Rao, ed., *Handbook of Statistics*, vol. 9: Computational Statistics, 662-721, Elsevier 1991.
- [6] Caillerie D., Homogenization of Periodic Media Tissued Composite Materials. *Proc. of Course on Mechanics of Composites. Theory and Simulation*. Technical University of Łódź, 1991.
- [7] Christensen R.M., *Mechanics of Composite Materials*. Wiley-Interscience, 1979.
- [8] Furmański P., Heat conduction in composites: homogenization and macroscopic behaviour. *Appl. Mech. Rev.* 50(6): 327-355, 1997.
- [9] Ghanem R.G., Spanos P.D., Spectral techniques for stochastic finite elements. *Arch. Comput. Meth. Engrg.* 4(1): 63-100, 1997.
- [10] Hammersley J.M., Handscomb D.C., *Monte Carlo Methods*. Wiley, 1964.
- [11] Hien T.D., Kleiber M., Stochastic finite element modelling in linear transient heat transfer. *Comput. Methods Appl. Mech. Engrg.* 144: 111-124, 1997.
- [12] Hurtado J.E., Barbat A.H., Monte Carlo techniques in computational stochastic mechanics. *Arch. Comput. Meth. Engrg.* 5(1): 3-30, 1998.
- [13] Kamiński M., Effective properties of random periodic fiber composites. *Proc. XIII Polish Conf. Comput. Methods Mech.*, Vol. II, pp. 599-606, Poznań, 1997.
- [14] Kamiński M., Homogenization in elastic random media. *Comput. Ass. Mech. & Engrg. Sci.* 3(1): 9-22, 1996.
- [15] Kamiński M., Hien T.D., Homogenization of the heat conduction problem in the fiber composites. *Arch. Mech.* (submitted).
- [16] Kamiński M., Kleiber M., Numerical homogenization of n-phase composites including stochastic interface defects. *Int. J. Num. Meth. Engrg.* (submitted).
- [17] Kamiński M., Kleiber M., Perturbation based stochastic finite element method for homogenization of two-phase elastic composites. *Comput. & Struct.* (submitted).
- [18] Kleiber M., Hien T.D., *The Stochastic Finite Element Method*. Wiley 1992.
- [19] Krishnamoorthy C.S., *Finite Element Analysis*, McGraw-Hill, 1994.

- [20] Pepper D.W., Heinrich J.C., *The Finite Element Method. Series in Computational and Physical Processes in Mechanics and Thermal Sciences*, Hemisphere 1992.
- [21] Rao H.S. et al., A model of heat transfer in brake pads by mathematical homogenization. *Sc. Engrg. Comp. Mat.* 6(4): 219-224, 1997.
- [22] Sab K., On the homogenization and the simulation of random materials. *Eur. J. Mech. Sol.* 11: 585-607, 1992.
- [23] Sanchez-Palencia E., *Non-homogeneous Media and Vibration Theory. Lectures Notes in Physics n° 127*, Berlin, Springer-Verlag, 1980.
- [24] Schellekens J.C.J., *Computational Strategies for Composite Structures*. TU Delft, 1992.
- [25] Suquet P., A dual method in homogenization: application to elastic media. *J. Mec. Theor. Appl.*, 79-98, 1982.

FIGURE CAPTIONS

- Fig. 1. Periodic fiber reinforced composite
- Fig. 2. The flowchart of the probabilistic simulation algorithm
- Fig. 3. Expected values of effective conductivity coefficient
- Fig. 4. Standard deviations of effective conductivity coefficient
- Fig. 5. Third order central probabilistic moments of effective conductivity coefficient
- Fig. 6. Fourth order central probabilistic moments of effective conductivity coefficient
- Fig. 7. Expected values of effective conductivity coefficients upper bounds
- Fig. 8. Expected values of effective conductivity coefficients lower bounds
- Fig. 9. Expected values of effective conductivity coefficients
- Fig. 10. Coefficients of variance of effective conductivity coefficients
- Fig. 11. Convergence of expected value of effective conductivity coefficient upper bound estimator
- Fig. 12. Convergence of expected value of effective conductivity coefficient estimator
- Fig. 13. Convergence of expected value of effective conductivity coefficient lower bound estimator
- Fig. 14. Convergence of variance coefficient of effective conductivity coefficient estimator
- Fig. 15. Convergence of assymetry coefficient of effective conductivity coefficient estimator
- Fig. 16. Convergence of concentration coefficient effective conductivity coefficient estimator
- Fig. 17. Heat conduction for the composite homogenized
- Fig. 18. Temperature field for upper bound of effective conductivity coefficient
- Fig. 19. Temperature field for effective conductivity coefficient
- Fig. 20. Temperature field for real composite structure
- Fig. 21. Temperature field for lower bound of effective conductivity coefficient

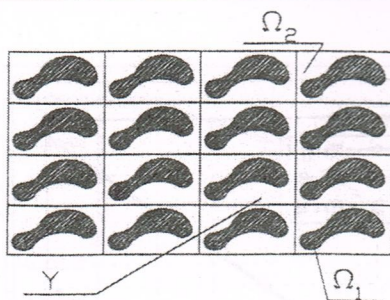


Fig. 1.

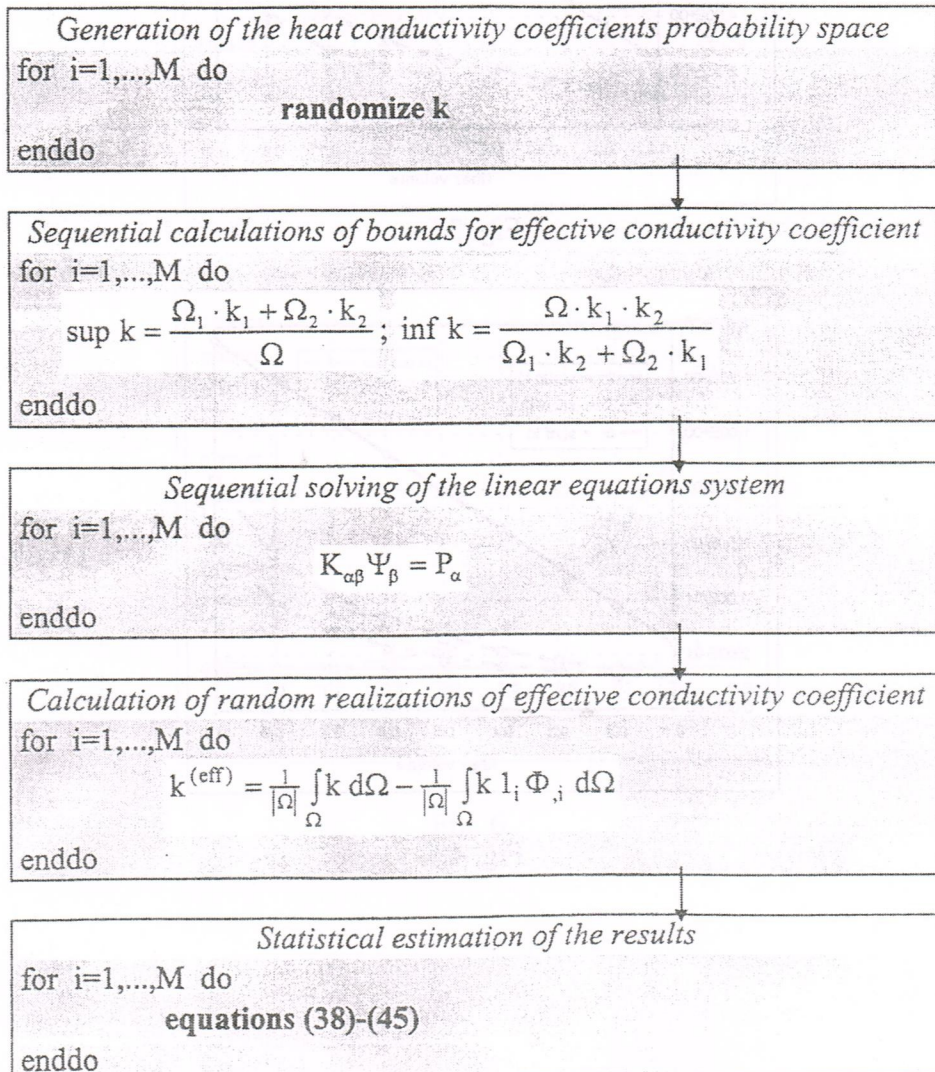


Fig. 2.

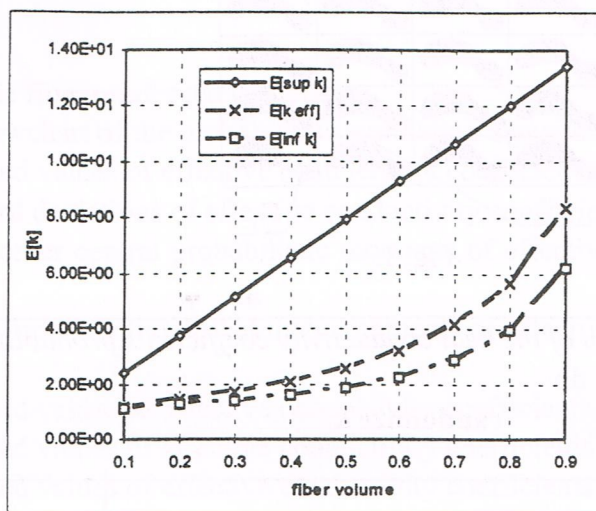


Fig. 3.

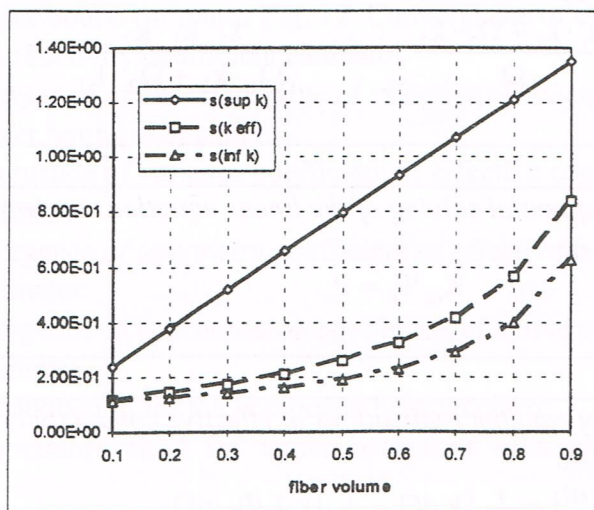


Fig. 4.

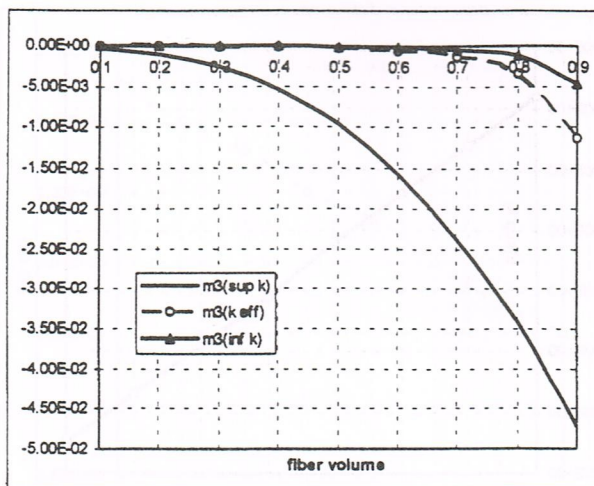


Fig. 5.

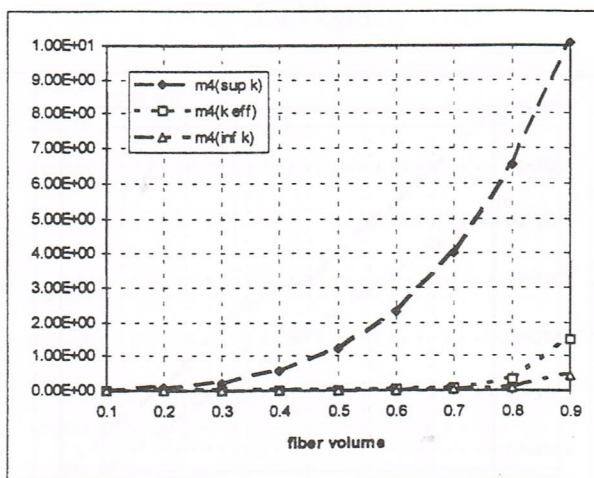


Fig. 6.

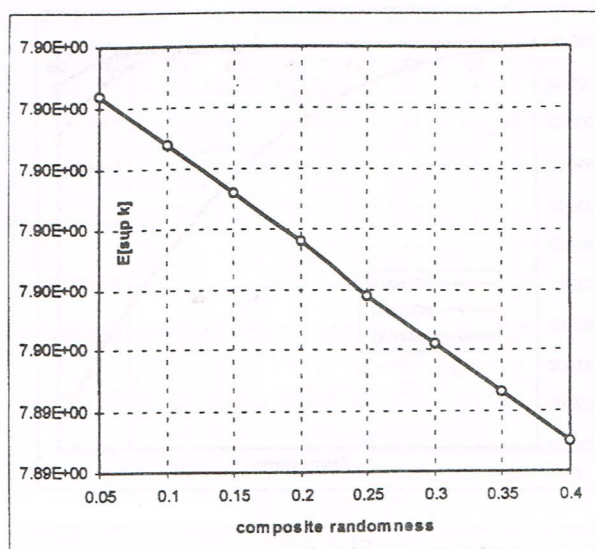


Fig. 7.

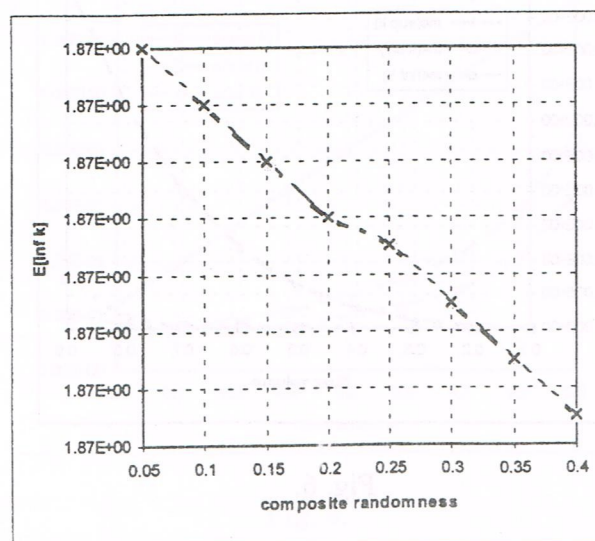


Fig. 8.

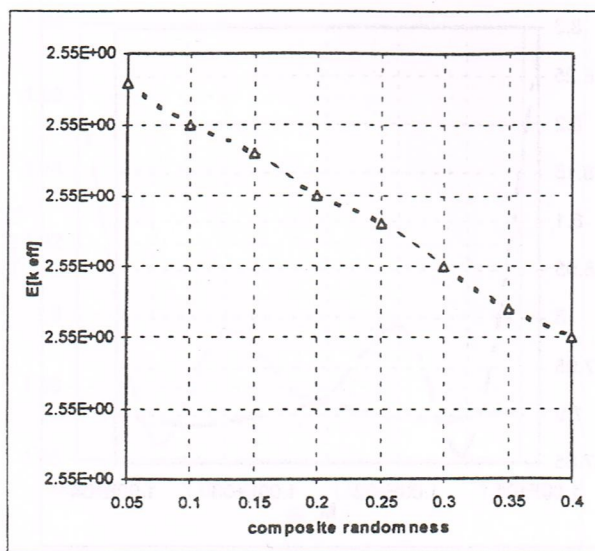


Fig. 9.

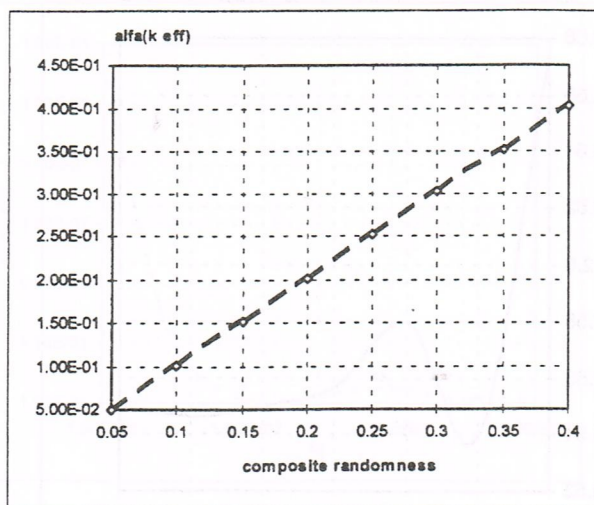


Fig. 10.

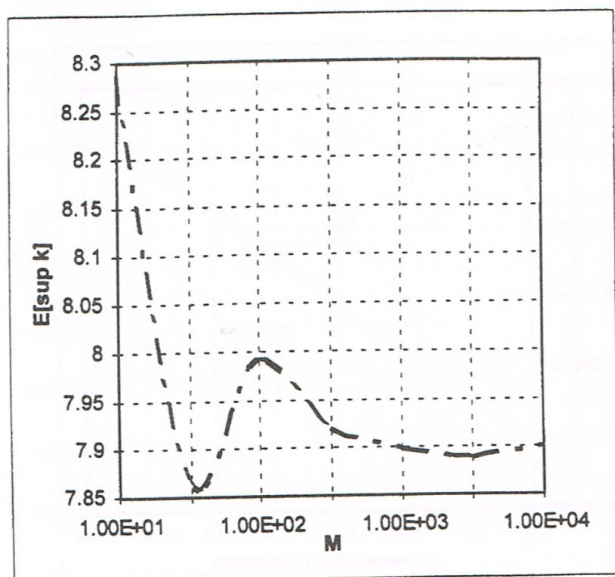


Fig. 11.

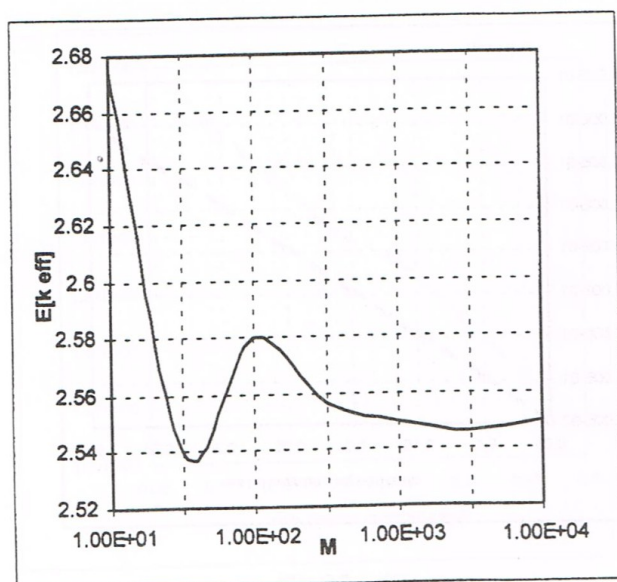


Fig. 12.

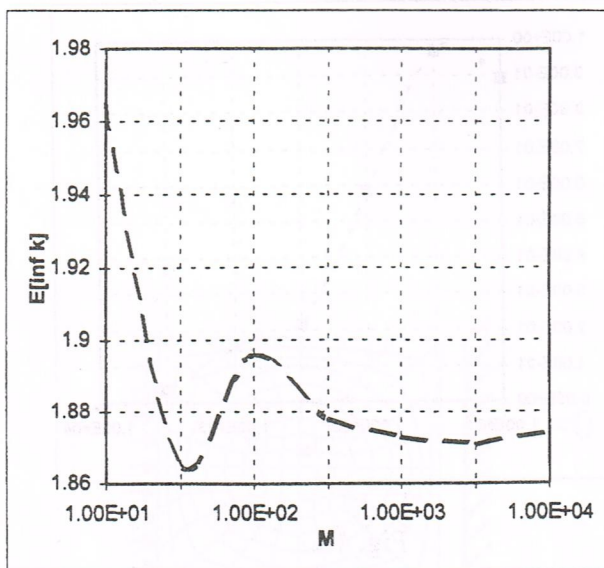


Fig. 13.

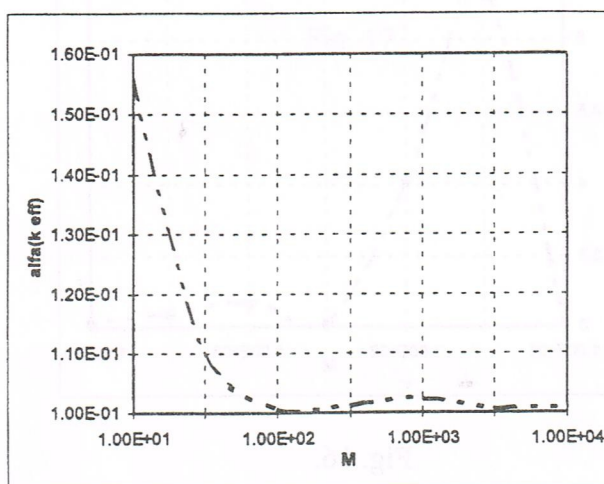


Fig. 14.

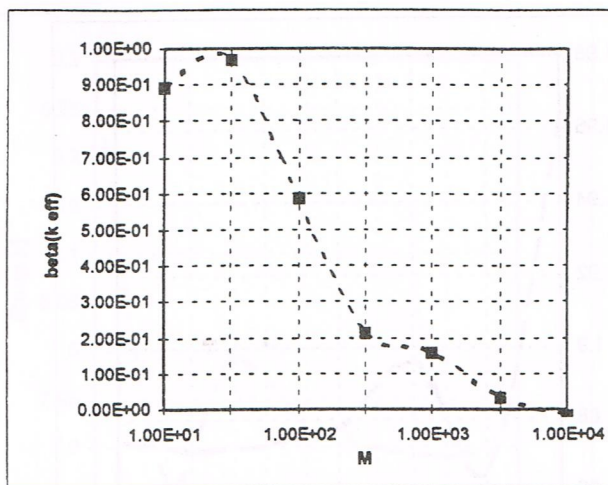


Fig. 15.

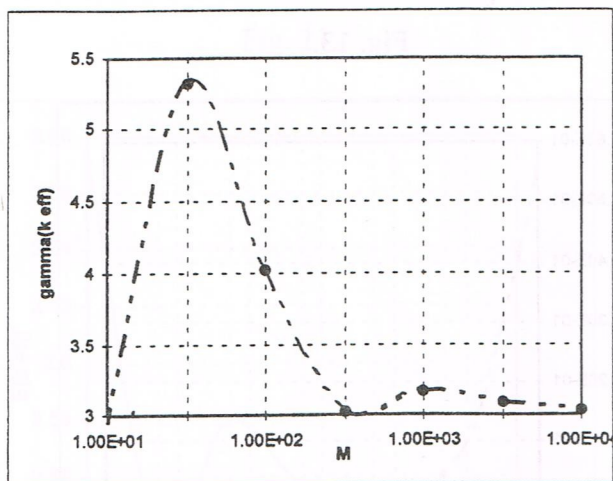


Fig. 16.

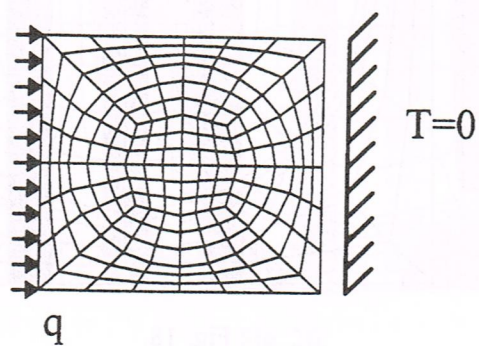
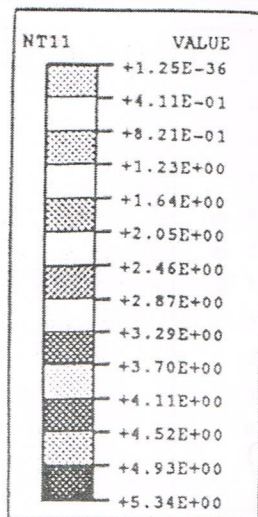


Fig. 17.



ABAQUS

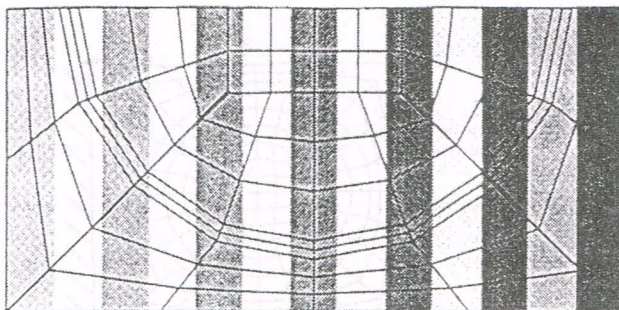
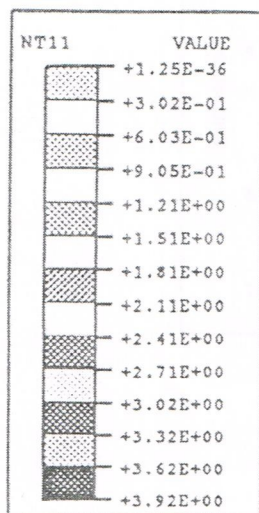


Fig. 18.



ABAQUS

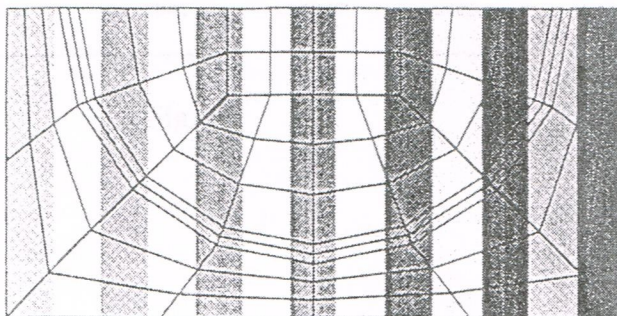
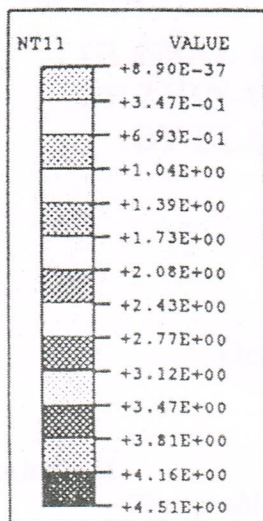


Fig. 19.



ABAQUS

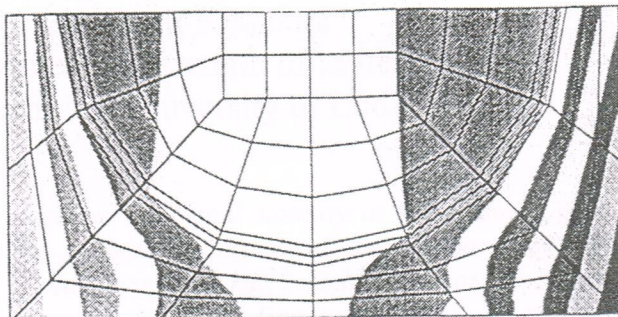
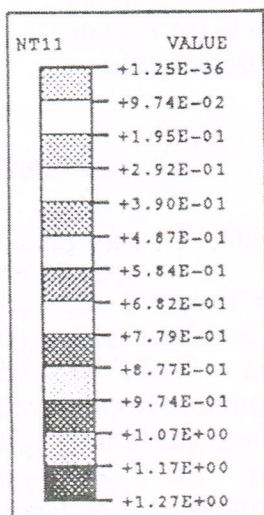


Fig. 20.



ABAQUS

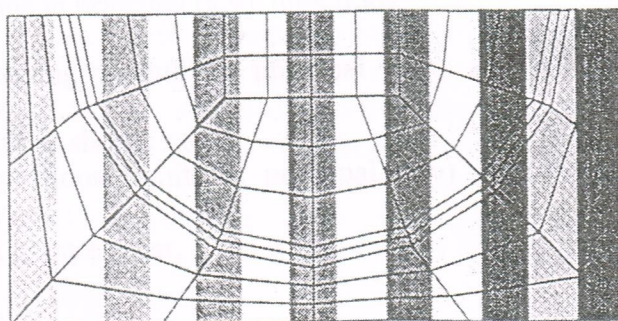


Fig. 21.