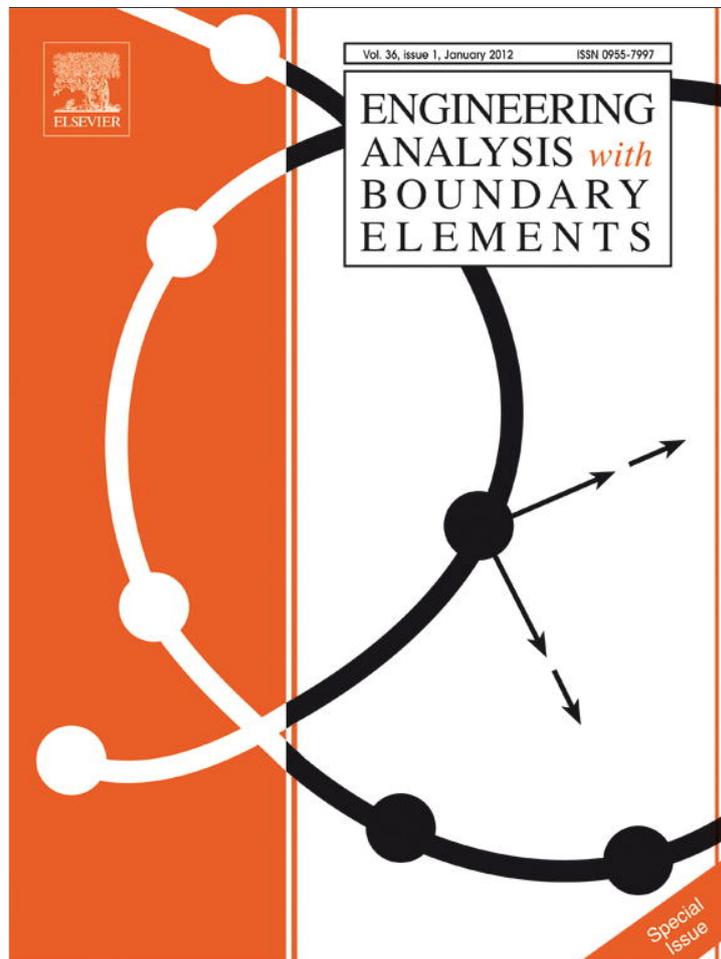


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Engineering Analysis with Boundary Elements

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Parallel computational models for composites reinforced by CNT-fibres

Vladimír Kompiš^{a,*}, Qing-Hua Qin^b, Zhuo-Jia Fu^c, C.S. Chen^d, Peter Droppa^a, Miroslav Kelemen^a, Wen Chen^c

^a Academy of Armed Forces, Liptovský Mikuláš, Slovakia

^b Australian National University, Canberra, Australia

^c Hohai University, Nanjing, China

^d Southern Mississippi University, Hattiesburg, USA

ARTICLE INFO

Article history:

Received 13 February 2011

Accepted 26 April 2011

Available online 23 August 2011

Keywords:

Composite materials

CNT-fibres

1D continuous Trefftz functions

LS collocation

Heat conduction

ABSTRACT

The aspect ratio of CNT-fibres reinforcing composite material is often with the value of $10^3:1-10^6:1$, or even larger. Thus, the method of Continuous Source Functions (MCSF) developed by authors using 1D continuous source functions distributed along the fibre axis enables to simulate the interaction of each fibre with the matrix and also with other fibres. 1D source functions can serve as Trefftz (T-) functions, which satisfy the governing equations inside the domain (matrix), and boundary conditions on the fibre–matrix interfaces are satisfied in collocation points in the least square (LS) sense along the fibre boundaries. The source functions are defined by Non-Uniform Rational B-Spline (NURBS). Because of large gradients of stress fields, large number of collocation points and many NURBS shape functions are necessary to simulate the interaction. Moreover, the matrices used for solving the problem are numerically full. In our model, only the interactions of each two fibres is solved by elimination and then the complex interaction of all fibres in a patch of fibres and the matrix is completed by iteration steps in order to increase efficiency of computations. Such procedure enables to use parallel algorithm for solving all interactions of the pairs of fibres parallel. For heat conduction problem, fibres are supposed to be super-conductive at the first stage. The energy balance condition in each fibre enables to find temperature change of each fibre by the interaction with the other fibre in the first iteration step. The next iteration step enables to correct the temperature changes of the fibres by complex interaction of all fibres and the matrix and distribution of the source functions inside the fibres are obtained. Temperatures and heat flows in the control volume enable then to define homogenised material properties for corresponding patch of the composite material.

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1. Introduction

CNT-fibres are widely used as reinforcing materials in most advanced composites [1]. According to Wikipedia the fibre classification in reinforced plastics fall into two classes: (i) CNT-fibres, also known as discontinuous fibres, with a general aspect ratio between 20 and 60, and (ii) long fibres, also known as continuous fibres, the general aspect ratio is between 200 and 500. However, in modern materials like polymers reinforced by Carbon Nano-Tubes (CNTs), where the diameter of the CNT is less than 20 nm and length more than 1 mm, is the very large aspect ratio and the cross sectional dimension does not satisfy the condition to be continuum for computational simulations, but the length is defined to be in the dimensions of micromechanics. Thus for the cross sectional dimension Molecular Dynamic (MD) should be

used. However, for studying the new material properties, reinforcing effect, conductivity and the longitudinal effect are the most important and aspect ratio of fibres is very large, but the fibre cannot be defined as long according to mechanical properties (local effects are very important for the mutual interaction of fibres and matrix).

In the past decades, fibre-reinforced composites have been widely used in engineering applications due to the superiority of their electro-thermo-mechanical (ETM) properties over the single matrix. Particularly, composite materials reinforced by CNT-fibres are often defined as materials of the future. Understanding the physical behaviour of these fibre-reinforced composites is essential for structural design.

Computational simulations can help in the understanding, analysis and design of these fibre-reinforced composite materials. Among the existing numerical methods, finite element method (FEM) [2,3], boundary element method (BEM) [4,5] and meshless methods [6] can be used for simulating the CNT-fibres behaviour. However, these classical numerical methods are suitable for the

* Corresponding author.

E-mail address: Vladimir.Kompiš@aos.sk (V. Kompiš).

lowest scale simulation only. It is worth noting that, in the CNT-fibres, the aspect ratio is often $10^3:1-10^6:1$, or even larger, which results in very large gradients localised in all ETM fields along the fibres and in the matrix. All the methods mentioned above require millions or even billions of equations after numerical discretization to obtain a sufficiently accurate solution of this kind of computer simulations.

Recently, the fast multipole method (FMM) [7] was developed to increase the efficiency of numerical models. The Fast Multipole Boundary Element Method (FMBEM) [8], which was used for simulation of these problems, reduces the computational cost for the far field interaction simulations; however, the classical BEM has to be used for simulating the near field interactions and the super-computers are necessary to solve the problem with good accuracy. The FMBEM is the only numerical method, which enables to solve the Representative Volume Element (RVE) of the matrix containing two to five thousand CNT-fibres (three to eleven million degrees of freedom (DOF)). The problems have been solved on super-computers, or on clusters of PC's [9–11].

More recently, Method of Continuous Source Functions (MCSF) developed in [12,13] using 1D continuous source functions distributed along the fibre axis enables to simulate interactions of a fibre with matrix and with other fibres very effectively. 1D continuous heat sources and heat dipoles distributed along fibre axes simulate the interaction among each pair of fibres with the matrix in some control volume (CV) for thermal problems. The inter-domain continuity between fibre and matrix are satisfied at collocation points on the fibre boundaries and so, the MCSF is a meshless method, which has some common features with the method of fundamental solution [14,15]. The computational domain in the model is the matrix in MCSF and the fibres are its outer part. It is supposed that the primary variables (temperature, displacements) as well their derivatives in the fibre axis direction (heat flow, stress, strain) are constant in the fibre cross sections. Thus, the source functions are outside of the domain.

However, in the CV all fibres interact with each other, which would lead to solution of very large system of equations. In the present models the matrix is split into sub-problems. The total system consists of sub-matrices simulating interaction of each fibre with the matrix and also with other fibres. In the sub-problems, we assume that the interaction of each fibre with the matrix and the interaction with one neighbour fibre only. Solving the much smaller sub-problems of a problem with N fibres we have to solve $N(N-1)/2$ sub-problems. Such procedure is also suitable for efficient parallel computing as the sub-matrices are independent of each other. The total changes in temperature are obtained by summing corresponding changes for each fibre with the iteration process.

This study will focus on heat conduction behaviour of composite materials reinforced by CNT-fibres with finite conductivity fibres. A brief outline of the paper is as follows: Section 2 describes the present model for heat conduction behaviour of composites reinforced by finite conductivity CNT-fibres. Then some conclusions and potential extensions of the proposed model are presented in Section 3.

2. Model description

Let us introduce the Method of Continuous Source Functions (MCSF) for analysing heat conduction behaviour of composite materials reinforced by CNT-fibres. We assume all matrix materials and fibres are homogeneous and isotropic and the dimensions of the matrix are infinite. To simulate heat conduction behaviour of composites reinforced by finite conductivity CNT-fibres (several order larger than matrix), the temperature and heat flow in all fibres should be obtained first. Heat flow can be calculated by

the source functions of unknown intensity, which can be solved from the inter-domain continuity (on the fibre–matrix interface).

For the simplicity of modelling all fields are split into two parts, the homogeneous part corresponding to the homogeneous problem of the matrix without fibres and local part containing the influence of interactions of fibres with the matrix. We will deal especially with the local fields in the composite material.

In the present model, the source functions (heat sources and heat dipoles) are 1D-continuously distributed along the fibre axis to simulate the interactions of fibres with the matrix and with other fibres in some control volume (CV) (Fig. 1). Heat source is a scalar quantity. Heat dipole is a heat source and heat sink acting at the same point by approaching each other in some coordinate direction. Mathematically, it is a derivative of the heat source in corresponding direction (i.e. the heat dipole is a vector).

Temperature field induced by a unit heat source acting in arbitrary point of infinite domain is the fundamental solution for heat problems and it is given by

$$T = \frac{1}{4\pi r} \quad (1)$$

where r is the distance of the field point t and source point s , where the heat source is acting at.

Temperature field induced by a unit heat dipole in the x_i direction is

$$T_{,i} = \frac{1}{4\pi} \left(\frac{1}{r} \right)_{,i} = -\frac{1}{4\pi r^2} r_{,i} = -\frac{1}{4\pi r^3} x_i \quad (2)$$

Heat flow in the x_i direction by the unit heat source (1) is given by

$$q_i = -k \frac{\partial T}{\partial x_i} = -k T_{,i} = k \frac{1}{4\pi r^3} x_i \quad (3)$$

where k is the heat conductivity of the matrix. Usually the heat conductivity of the fibre is several orders higher than that of the matrix and it is 1000 times higher in the example of this study.

Note that the heat flow is influenced not only by the source function in the corresponding fibre, but also with the source functions located in all neighbour fibres.

Similarly the heat flow by the dipole (2) is obtained from the second derivative of (1)

$$T_{,ij} = \frac{1}{4\pi r^3} \left(\frac{3x_i x_j}{r^2} - \delta_{ij} \right) \quad (4)$$

where is the δ_{ij} Kronecker delta.

Heat flow through a surface with the normal n is defined as

$$q_n = q_i n_i \quad (5)$$

Collocation points (Fig. 1) are located on the interface between fibre and matrix. Then the intensities of the source functions can be computed by satisfying the inter-domain boundary

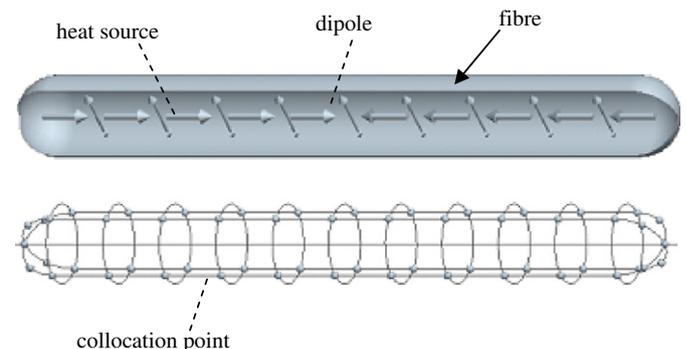


Fig. 1. Distribution of source functions and collocation points.

(continuity) conditions in collocation points on the fibre–matrix interface boundaries. In the present method, four collocation points are used on each cross-section of the fibre for satisfying the boundary (continuity) conditions in the perpendicular direction of the fibre–matrix interface boundary. It should be stressed that the ends of a fibre should be in the form of half spheres or cylinders. It is important to satisfy the boundary conditions (BCs) in these parts as well. Without considering these BCs, the source functions located along the fibre axis may lead to incorrect results in evaluation of the heat conduction behaviour.

In order to find the unknown intensities of the source functions, we have to solve 1D quasi-singular equation in the form

$$\int_r K(s,t)f(t)d\Gamma = g(s) \quad (6)$$

where $K(s,t)$ is the kernel function, which is the corresponding source function in our case, $f(t)$ is the unknown intensity of the source function, $g(s)$ is the function prescribing the BC and Γ is the 1D integration curve along fibres' axes.

Numerical integration along 1D elements and the corresponding Non-Uniform Rational B-Spline (NURBS) shape functions [16,17] performed as the integrands in Eq. (5) are quasi-singular and complicated for analytical evaluation if the fibres are curved. After numerical experiments on behaviour of source functions in composite material and on their influence on physical fields, the following conclusions are drawn for generation of collocation points and numerical integration: very fine points defining NURBS for source functions are to be chosen in the end parts of the fibres because of large gradients in all fields in fibres and matrix. As there are very large differences in the denominator (distance between source and collocation points) the whole integration path is split into integration elements. In our models the smallest element (closest to the collocation point) has to be equal to the fibre diameter and the others are about as large as the distance of its closest point from the collocation point. In this way same number of Gauss integration points can be used for all elements with about equal numerical error from all integration elements in the model. The 5 point Gauss quadrature is enough to give good accuracy in this case.

Usually less than 100 equations are enough to simulate the inter-domain continuity for one fibre. However, if the model contains large number of fibres, the model would be large due to the large number of system equations and the computation time would last a very long time. According to the basic mechanical principle, the matrix in the proposed model is split into sub-problems to increase the efficiency of computations. The total system consists of sub-matrices simulating interaction of each fibre with the matrix and also of the fibre with each other. If there are N fibres in the control-volume model (CV), then it is necessary to solve the interaction of $N(N-1)/2$ pairs of fibres. In the sub-problems, there is the interaction of each fibre with the matrix and the interaction with only one neighbour fibre. This reduces computational time and also requirements on the memory. Moreover, as the sub-matrices are independent of each other, the model is suitable for efficient parallel computing [18] (we use parallel MATLAB for the numerical simulations). The total changes of temperature are obtained by summing corresponding changes for each fibre. Then the complex interaction of all fibres in a patch of fibres and the matrix is completed by iteration steps.

Therefore, the present model can be divided into three steps. In the first two steps, it is supposed that fibres are superconductors and so, the temperature gradient of each fibre is constant. The temperature distributions in the whole patch of fibres are computed from the interaction of all fibres by the iteration process in the first step. Then the intensities of source function together with the temperature in all fibres are corrected by the

iteration process. Finally, removing the superconductivity assumption, the present method calculates the temperature and intensities of the source function for composites reinforced by finite conductivity CNT-fibres, then temperature and heat flow on the homogeneous matrix around the fibres are obtained in this way.

In the example a patch of regularly distributed overlapped $N=23$ fibres with aspect ratio 100:1 are computed in a PC. Fig. 2 shows one plane of a patch of overlapping rows of fibres (similar structure is in x_2x_3 plane, i.e. the patch in Fig. 2 would contain 113 fibres). Radius of fibres is 1, distance between layers of fibres in perpendicular direction is 4 and distance between fibres in fibre direction is 10.

Step 1: consider the interaction of two fibres (I and J) in one sub-problem. To satisfy the inter-domain continuity, the following expression can be obtained by solving the problem (5) numerically

$$A_s c = b \quad (7)$$

where the interpolation matrix A_s can be easily obtained from the heat source and heat dipole calculated by source points and collocation points on the two corresponding fibres. It is necessary to solve the system of equation with 3-column rhs, i.e. b is a 3-column matrix. The first column is the temperature (T_b) on the collocation points to satisfy the inter-domain continuity, which are used to compute the corresponding intensities of heat source and heat dipole (c_{ij}), and the other two with constant temperature equal 1 in one fibre and 0 in the other fibre to obtain the intensities of heat source and heat dipole intensities (c_{10} and c_{01}) in both fibres for producing unit temperature in one fibre. From the total heat flow in each fibre change in temperature of each fibre is obtained so that the total heat flow in each fibre is equal to zero, as no fibre can generate any heat. Therefore, the intensities of source functions $c = [c_{ij} \ c_{10} \ c_{01}]$ is also a 3-column matrix. It should be mentioned that temperature (T_b) can be split into homogeneous part T_H (matrix without fibres) and local part T_L . According to the fibre superconductivity assumption, the temperature T_H is linearly distributed along fibres, if the fibres are straight, with opposite temperature gradient t_g to that of the homogeneous field, where $t_g=1$ in this study. T_L is the temperature change obtained from the interaction of fibres with the matrix by the iterative process.

In addition, it is assumed that the temperature in a cross-section of the fibre is constant (if the fibre is a superconductor, this assumption is exact). This condition is prescribed in the form that differences of temperature are zero in opposite points in the cross-section of the fibre.

$$A_c c = 0 \quad (8)$$

where A_c is constructed from the difference of source functions between the two opposite collocation points in the same cross-section of the fibre. Combining Eqs. (7) and (8), the final system of

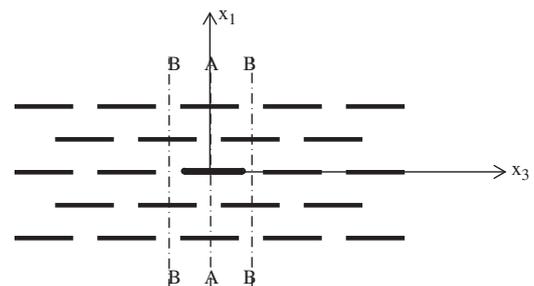


Fig. 2. Patch of overlapping rows of fibres.

inter-domain continuity problem can be rewritten as follows:

$$Ac = \begin{bmatrix} A_s \\ A_c \end{bmatrix} c = \begin{bmatrix} b \\ 0 \end{bmatrix} \quad (9)$$

Recall that the vector c contains intensities of both heat source and heat dipoles directed in two perpendicular directions to the fibre axis along the fibre axis.

Obtaining the intensities of source functions from Eq. (9), the heat flow through the fibre–matrix interface on collocation points of fibres can be computed as

$$q = B_s c \quad (10)$$

where B_s is the matrix corresponding to A_s by employing Eqs. (3)–(5) for heat sources and heat dipoles.

Integrating the heat flow through the fibre–matrix interface along each fibre, the corresponding heat flows ($HF_{ij}(I)$, $HF_{10}(I)$, $HF_{01}(I)$ for fibre I ; $HF_{ij}(J)$, $HF_{10}(J)$, $HF_{01}(J)$ for fibre J) are computed. The three values correspond to the three rhs for each fibre. Thus, the temperature changes (T_i and T_j) in each fibre in the corresponding iteration are found from the energy balance in both fibres as

$$\begin{bmatrix} HF_{10}(I) & HF_{01}(I) \\ HF_{10}(J) & HF_{01}(J) \end{bmatrix} \begin{bmatrix} T_i \\ T_j \end{bmatrix} + \begin{bmatrix} HF_{ij}(I) \\ HF_{ij}(J) \end{bmatrix} = 0 \quad (11)$$

Similarly, by summing the corresponding heat flow of each fibre computed from the interaction of each pair of fibres, the change in temperature $T_i(k)$ in each fibre is obtained from the energy balance in all fibres, where i denotes the i th iteration step and $k=1, \dots, N$ fibres. In this step, we implement the iteration process to correct the value $T_L = T_i(I) - T_i(J)/2$ into the right hand side of system (9), the change in temperature in the middle of the corresponding pair of fibres.

To accelerate the convergence rate, the following expression has been employed after three iterations

$$\frac{T_1 - T_e}{T_1 - T_2} = \frac{T_2 - T_e}{T_2 - T_3} \quad (12)$$

where T_i ($i=1,2,3$) denotes temperature in the whole patch of fibres in the i th iteration step, and T_e the temperature change in the whole patch of fibres by implementing expression (12).

In the next iteration step, the temperature distribution of fibres T_4 does not change so much with T_e . This reveals the efficiency of the expression (12).

Step 2: after achieving the convergent result in Step1 (four iteration steps are enough), the intensities of source function together with the temperature in all fibres are corrected in further iterations. As the effects of the temperature changes in each fibre are considered, the intensities of source function should be modified by the following expression:

$$c_m = c_{ij} + c_{10}T_i + c_{01}T_j \quad (13)$$

Then consider the interaction of all pairs of fibres, the total intensities of heat source (C_T) and heat dipole (C_D) can be obtained by summing the corresponding intensities of source function computed from the interaction of each pair of fibres. Furthermore the temperature distribution TIJ on the collocation point in each fibre with the interaction of all pairs of fibres can be summed from the corresponding temperature distribution multiplying the total intensities of heat source (C_T) and heat dipole (C_D) by the interpolation matrix A_s . However, these temperatures and intensities of source function cannot get the correct temperature gradients in each fibre ($-t_g$), where the difference is a constant. The further correction is to find this constant k_0 . By using the

definition of temperature gradient in the fibre, we can get

$$-k_0 t_g = \frac{(TIJ(i_c, I) + TIJ(i_c + nc, I) + TIJ(i_c + 2nc, I) + TIJ(i_c + 3nc, I))\Delta z - 4T_c \Delta z}{z(i_c)\Delta z} \quad (14)$$

where nc denotes the number of collocation points along the fibre in one side of the fibre, namely, totally $4nc$ collocation points are placed on the fibre surface. T_c is the temperature in the centre of the fibre, $z(i_c)$ stands for the placement of i_c th collocation point in the fibre axis, $\Delta z = z(i_c + 1) - z(i_c - 1)$, $i_c = 2, 3, \dots, nc - 1$. It should be mentioned that there are only two unknowns (T_c and k_0) and $nc - 2$ equations in one fibre. The unknowns can be easily solved by the Least squares approach. Thus all the values (C_T , C_D , TIJ and T_c) are corrected by dividing k_0 . It is worth noting that the temperature change T_L for computing the intensities in the next iteration should be corrected by taking into account T_c and T_i , T_j

$$T_L = \frac{T_{i-1}(I) - T_{i-1}(J) + T_i - T_j + T_c(I) - T_c(J)}{2} \quad (15)$$

Iterate the above computation in several steps (two iterations in this example), the final temperature and intensities of source functions for composites reinforced by superconductivity CNT-fibres can be achieved.

Step 3: in this step, the assumption of the fibre superconductivity is removed, we set the heat conductivity of fibres is 1000 times higher than that of the matrix. The corresponding temperature and intensities of source function should be corrected by the iteration process. The simple way is similar to Step 2 that finding the correction difference coefficients (CDs) to guarantee “ $-t_g$ ” temperature gradients in each fibre in all iterations.

By integrating the intensities of heat source (C_T) with the corresponding NURBS function along 1D elements in the fibre, the heat flow (H_F) in the fibre can be obtained. Moreover, the fibre temperature (T_F) on the NURBS interpolation points x_i obtained from the source function of the fibre can be calculated as

$$T_F(x_i) = \frac{1}{1000} \sum_{j=2}^i \frac{1}{2} (H_F(j) + H_F(j-1))(x_j - x_{j-1}) \quad (16)$$

Furthermore, the temperature in fibres can be approximated by polynomial series, 8 terms are used in this study.

$$T(x) = a_0 + \sum_{j=1}^7 a_j x^j \quad (17)$$

where x is the location of the points in the fibre axis, a_0, a_j ($j=1, 2, \dots, 7$) are the unknown coefficients of polynomial expansion, and these unknowns can be found by inserting the fibre temperature (T_F) on the NURBS interpolation points x_i into expression (17). Therefore, the temperature T_5 on the collocation points of fibre can be evaluated as

$$T_5(z) = a_0 + \sum_{j=1}^7 a_j z^j \quad (18)$$

and the corresponding temperature gradients of the fibre t_G can be calculated from

$$t_G = \frac{T_5(z) - a_0}{z} = \sum_{j=1}^7 a_j z^{j-1} \quad (19)$$

Finally, the correction difference coefficients (CDs) are the difference between t_G and t_g .

$$CD = \frac{t_g}{t_G} \quad (20)$$

It is worth noting that the temperature gradient is not equal to opposite t_g , where the corrected temperature gradient should be opposite t_G . Moreover, the temperature along fibres, which is

constant for hyper-conductivity (and the local field is linear along the fibre) changes along the fibre. This change, of course will decrease the reinforcing effect of real fibres comparing to the problem of infinite conductivity.

By implementing several iterations, the final corrected fibre temperature (\bar{T}_F), heat flow (\bar{H}_F) and intensities of source function (\bar{C}_T, \bar{C}_D) in the fibre can be obtained. Then the temperature distribution and heat flow of the homogenisation matrix around the fibres can be calculated using the final corrected intensities of source function \bar{C}_T, \bar{C}_D . For homogenisation of the problem with regularly distributed fibres the matrix around fibre can be split into three regions. Taking into account of the matrix around fibre I , Fig. 3 plots the corresponding matrix around fibre I (the domain inside the dash-dotted line) and three corresponding splitting regions (R_1, R_2, R_3). Due to the symmetry property, half of the matrix around fibre ($x_3 > 0$) is considered in the computation. The Control Volume Element (CVE) consists of the three regions and temperature and heat flow are integrated through the CVE surface. The present method discretizes each region into elements as defined by the three regions. Gauss integration scheme has been used to obtain the fields using 4×4 gauss points in each element. Fig. 4 shows the

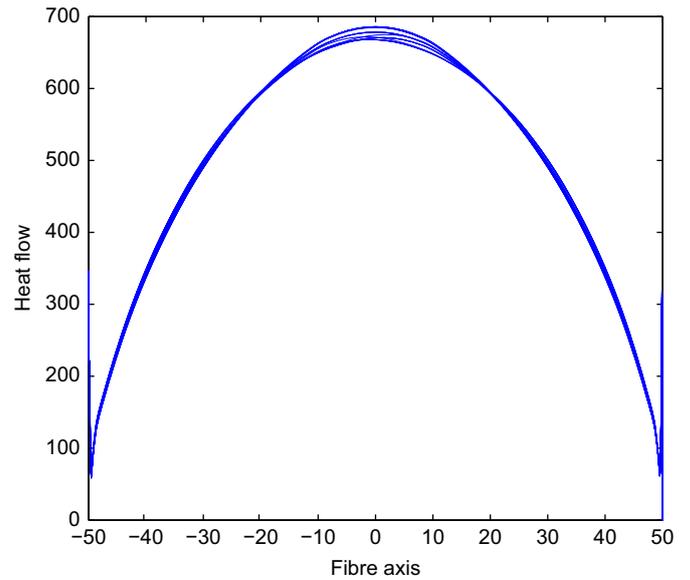


Fig. 5. Heat flow along fibres.

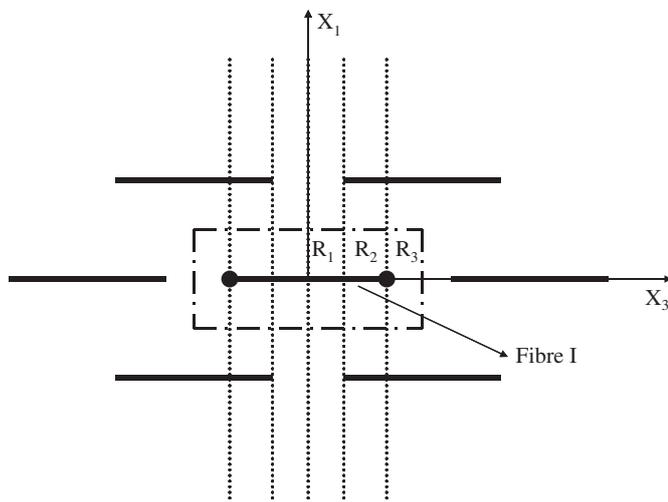


Fig. 3. Matrix around fibre I (the domain inside the dash-dotted line) and three corresponding splitting regions (R_1, R_2, R_3).

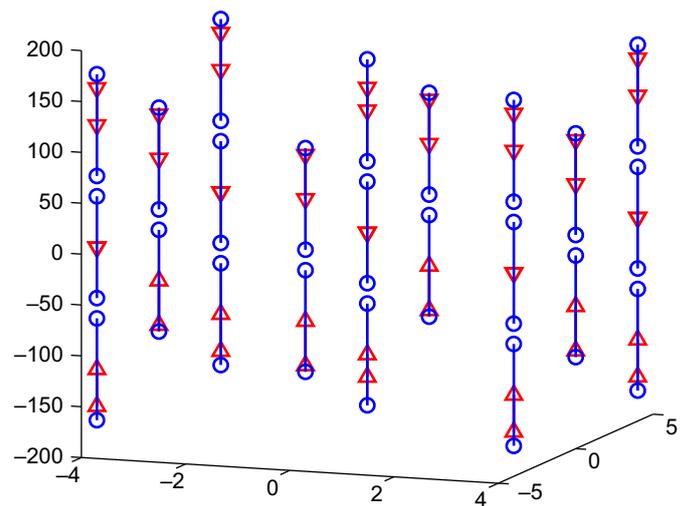


Fig. 6. Temperature increase/decrease in the central points of fibres.

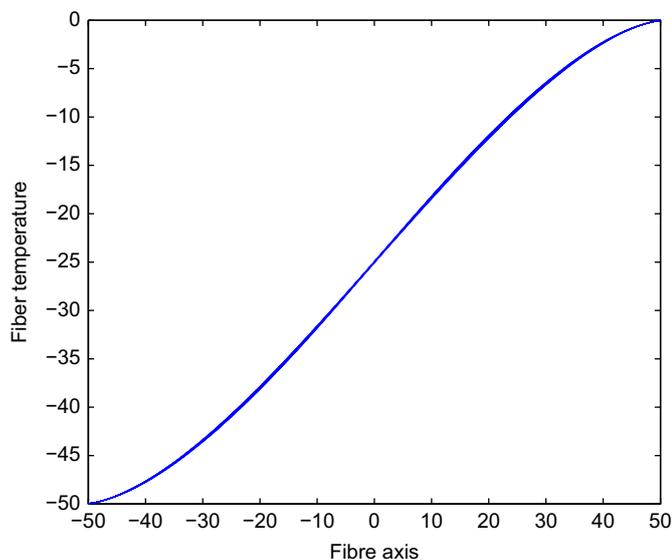


Fig. 4. Temperature along a fibre for finite conductivity of fibres.

temperature distribution along a fibre for finite conductivity of fibres. Recall that the distribution is linear for hyper-conductive fibres. Fig. 5 presents the heat flow in fibres for such composite material and Fig. 6 gives temperature increase/decrease in the central points of fibres comparing to the homogeneous material for a patch of 23 regularly distributed fibres with the overlay as indicated in Fig. 3.

3. Conclusions

The present model employs the solution of sub-problems and iterative steps to obtain a complete solution for interaction of many fibres reinforcing composite material with finite conductivity of fibres. Numerical results demonstrate that the present model improves the efficiency of the MCSF. Quasi-singular integral equations describing the behaviour are solved by collocation in points on the fibre–matrix interface.

All fields are split into two parts that one is corresponding to homogeneous material and another is local field corresponding to

the interaction of fibre with matrix and with other fibres. The interaction of each of the two fibres is solved by the elimination process only, and the complex interaction of all fibres in a patch of fibres and the matrix is completed by iteration steps. Energy balance is used to obtain temperature change in a pair of fibres in the interaction with the matrix in the elimination process and temperature change in the fibres centres and source functions distribution along fibres are iteratively improved for the interaction of the complex patch of fibres in the CVE first for super-conductive material of the fibres and then the finite conductivity of fibres is included into the iteration process.

This kind of computer simulation is very suitable for parallel computing. This is even more important in elasticity problems, as the number of equations to solve a similar problem to that of the heat transfer is three times larger and computer time increases then by nearly one order. Rigid body displacements of fibres correspond to the temperature of the super-conductive fibre. Displacements correspond to temperature and as they are vectors with 3 components in 3D, the problem is more complicated and takes more CPU time. Force dipoles and couples in two directions perpendicular to the fibre axis are necessary to satisfy the inter-domain boundary conditions instead of one component of heat dipole in heat transfer [12].

The primary and secondary fields, i.e. temperature and heat flow in heat problems, in the CVE boundary can be used for homogenisation [19–21].

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