ELEMENT FREE GALERKIN METHOD FOR TRANSIENT THERMAL ANALYSIS OF CARBON NANOTUBE COMPOSITES

by

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This paper deals with the transient thermal analysis of carbon nanotube composites via meshless element free Galerkin method. A three-dimensional representative volume element containing single nanotube has been taken as model for these simulations. Essential boundary conditions have been enforced via penalty approach. Simulations using continuum mechanics have been carried out for two different values of nanotube length. Backward difference and Galerkin approaches have been utilized for time approximation, and the results obtained by backward difference method are compared with those obtained by Galerkin approach.

Key words: *carbon nanotube, nano-composites, continuum mechanics, transient thermal analysis, meshless, element free Galerkin method*

Introduction

Carbon nanotubes (CNTs), due to their unique structure, remarkable properties and wide range of applications, have attracted much attention in recent years [1-5]. Carbon nanotube reinforced composites is one of their many applications.

Thermally and electrically conductive polymer composites are widely used in the electronics, automotive, and aerospace industries to dissipate heat and prevent the storage of static charge. Carbon fibers or copper wires are typically used as fillers for this purpose; however the requirement of high loadings often produces the harmful effect on the mechanical properties of the matrix. Therefore, high aspect ratio and highly conductive materials such as CNTs are regarded as promising fillers due to their superior properties as compared to conventional carbon fibers. The rapid advancement in the bulk synthesis of CNTs makes it possible to produce CNTs-based composites. Many believe that the reinforcement of CNTs in polymer matrix may provide us an entirely new class of materials. Therefore, the study of thermal behavior of carbon nanotube composites becomes an obvious choice. In past, some studies based on numerical simulations have been carried out to predict the thermal properties of nano-composites using continuum mechanics approach [6-12]. Nishimura and Liu [6] applied the boundary integral equation method for prediction the thermal behavior of CNT based nano-composites. They solved a heat conduction problem in 2-D infinite domain embedded with many rigid inclusions by fast multipole boundary element method. Zhang *et al*. [7-8] used the meshless hybrid boundary node method for the thermal simulation of carbon nanotube composites. Song and Youn [9] evaluated the effective thermal conductivity of the carbon nanotube/polymer composites by control volume finite element method. Singh *et al*. [10-12] applied the meshless element free Galerkin method to study the thermal behavior of CNT-composites. Ang *et al.* [13] assumed that CNT behaves as a thermal superconductor inside polymer matrix for the thermal analysis of carbon nanotube composites, and developed an analytical solution using Bessel functions.

CNTs and their composites may have various applications in near future where it's necessary to study their transient behavior before real engineering and industrial applications such as electrodes in gas discharge tubes, solid state devices (diode, transistor, MOSFET), electrical elements (resistor, inductor, and capacitor) but so far, the numerical studies were limited to predict the steady-state thermal behavior of CNT-composites [6-12]. Therefore, in the present work, mesh-free element free Galerkin method has been applied for the transient thermal simulation of CNT-composites. Nanoscale square representative volume element (RVEs) containing single CNT have been taken for thermal analysis. Time approximation has been performed by backward difference and Galerkin approaches, and the results obtained by backward difference method are compared with those obtained by Galerkin approach.

Review of element free Galerkin method

The discretization of governing equations by element free Galerkin (EFG) method requires a moving least square (MLS) approximation scheme, which consist of three components: a weight function associated with each node, a basis function, and a set of non-constant coefficients. Using MLS approximation scheme, an unknown function of temperature $T(x)$ is approximated with $T^h(x)$ given by [10-12]:

$$T^h(x) = \sum_{i=1}^{n} \Phi_i(x) T_i = \Phi(x) T \tag{1}$$

where, $\mathbf{x}^T = [x, y, z]$, T_i are nodal parameters, and $\Phi_i(x)$ is the shape function, which is defined as:

$$\Phi_i(x) = \sum_{j=1}^{m} p_j(x) \left(\frac{B(x)}{A(x)} \right)_{ji} = p^T \frac{B_i}{A} \tag{2a}$$

where

$$A(x) = \sum_{i=1}^{n} w(x - x_i) p(x_i) p^T(x_i) \tag{2b}$$

$$B(x) = [w(x - x_i) p(x_1),\ w(x - x_2) p(x_2), \ldots, w(x - x_n) p(x_n)] \tag{2c}$$

The cubicspline weight function [14] has been used in this work, which is given as:

$$f(s) = \begin{cases} \frac{2}{3} - 4s^2 + 4s^3 & s \le \frac{1}{2} \\ \frac{4}{3} - 4s + 4s^2 - \frac{4s^3}{3} & \frac{1}{2} < s \le 1 \\ 0 & s > 1 \end{cases} \tag{3a}$$

where s is the normalized radius.

At any point x, a tensor product weight function is computed as:

$$w(x - x_i) = f\left(\frac{|x - x_i|}{d_{mxi}} \right) f\left(\frac{|y - y_i|}{d_{myi}} \right) \tag{3b}$$

where $d_{mxi} = d_{max} c_{xi}$, $d_{myi} = d_{max} c_{yi}$, $d_{mzi} = d_{max} c_{zi}$, d_{max} = scaling parameter that defines the size of the domain of influence, and c_{xi}, c_{yi}, and c_{zi} at node i are the distances to the nearest neighbors denoted by $c_{xi} = \max_j |x_i - x_j|$, $c_{yi} = \max|y_i - y_j|$, and $c_{zi} = \max_j |z_i - z_j|$. The full details of EFG method can be found in [15].

Numerical implementation

A square RVE containing single nanotube (fig. 1) have been taken as a model for the transient thermal analysis of carbon nanotube composites. Perfect interface has been assumed between nanotube and polymer matrix in the present simulations. The nanotube has been placed in square RVE such that the axis of nanotube coincides with the axis of square RVE. Two opposite surfaces of the RVE are maintained at two different constant temperatures *i. e.* T_1 and T_2 respectively, while other surfaces are kept insulated.

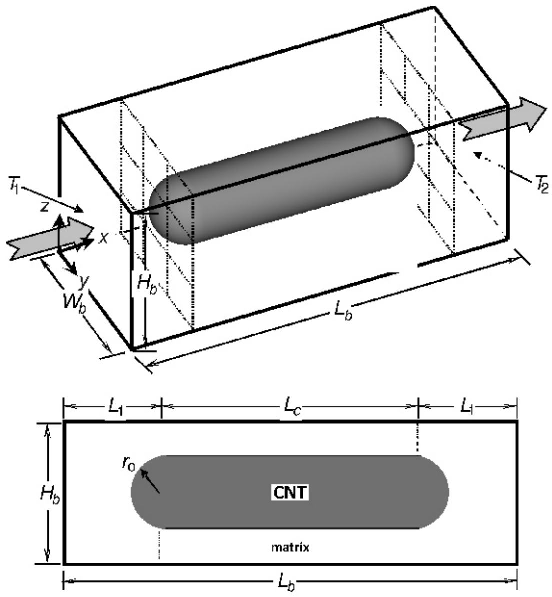

Figure 1. CNT-composite model along with its dimensions

The governing heat conduction equation in Cartesian coordinate system is given as:

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) = \rho c\frac{\partial T}{\partial t} \tag{4a}$$

along with following essential boundary conditions:

$$T(0,y,z) = T_1 \tag{4b}$$

$$T(L,y,z) = T_2 \tag{4c}$$

The weighted integral form of eq. (4a) is given as:

$$\int_{V_m} \tilde{w}\left[\frac{\partial}{\partial x}\left(k_m\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_m\frac{\partial}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_m\frac{\partial T}{\partial z}\right) - \rho c\dot{T}\right] \mathrm{d}V$$

$$+ \int_{V_c} \tilde{w}\left[\frac{\partial}{\partial x}\left(k_c\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_c\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_c\frac{\partial T}{\partial z}\right) - \rho c\dot{T}\right] \mathrm{d}V = 0 \tag{5}$$

Using divergence theorem, the weak form of eq. (5) is obtained as:

$$\int_{V_m}\left(\frac{\partial \tilde{w}}{\partial x}k_m\frac{\partial T}{\partial x}+\frac{\partial \tilde{w}}{\partial y}k_m\frac{\partial T}{\partial y}+\frac{\partial \tilde{w}}{\partial z}k_m\frac{\partial T}{\partial z}+\tilde{w}\rho_m c_m\dot{T}\right)\mathrm{d}V + \int_{V_c}\left(\frac{\partial \tilde{w}}{\partial x}k_c\frac{\partial T}{\partial x}+\frac{\partial \tilde{w}}{\partial y}k_c\frac{\partial T}{\partial y}+\frac{\partial \tilde{w}}{\partial z}k_c\frac{\partial T}{\partial z}+\tilde{w}\rho_c c_c\dot{T}\right)\mathrm{d}V = 0 \tag{6}$$

From eq. (6), the functional I(T) can be obtained as:

$$I(T)=\int_{V_m}\frac{1}{2}\left[k_m\left(\frac{\partial T}{\partial x}\right)^2+k_m\left(\frac{\partial T}{\partial y}\right)^2+k_m\left(\frac{\partial T}{\partial z}\right)^2\right]\mathrm{d}V+\int_{V_m}\rho_m c_m T\dot{T}\,\mathrm{d}V + \int_{V_c}\frac{1}{2}\left[k_c\left(\frac{\partial T}{\partial x}\right)^2+k_c\left(\frac{\partial T}{\partial y}\right)^2+k_c\left(\frac{\partial T}{\partial z}\right)^2\right]\mathrm{d}V+\int_{V_c}\rho_c c_c T\dot{T}\,\mathrm{d}V \tag{7}$$

Enforcing essential boundary conditions using penalty method, the functional I^*(T) is obtained as:

$$I^*(T)=\int_{V_m}\frac{1}{2}\left[k_m\left(\frac{\partial T}{\partial x}\right)^2+k_m\left(\frac{\partial T}{\partial y}\right)^2+k_m\left(\frac{\partial T}{\partial z}\right)^2\right]\mathrm{d}V+\int_{V_m}\rho_m c_m T\dot{T}\,\mathrm{d}V + \int_{V_c}\frac{1}{2}\left[k_c\left(\frac{\partial T}{\partial x}\right)^2+k_c\left(\frac{\partial T}{\partial y}\right)^2+k_c\left(\frac{\partial T}{\partial z}\right)^2\right]\mathrm{d}V+\int_{V_c}\rho_c c_c T\dot{T}\,\mathrm{d}V + \frac{\tilde{\alpha}}{2}\int_{S_1}(T-T_1)^2\,\mathrm{d}S+\frac{\tilde{\alpha}}{2}\int_{S_2}(T-T_2)^2\,\mathrm{d}S \tag{8}$$

Taking variation of I^*(T), eq. (8) is written by:

$$\delta I^*(T)=\int_{V_m}\left[k_m\left(\frac{\partial T}{\partial x}\right)^T\delta\left(\frac{\partial T}{\partial x}\right)+k_m\left(\frac{\partial T}{\partial y}\right)^T\delta\left(\frac{\partial T}{\partial y}\right)+k_m\left(\frac{\partial T}{\partial z}\right)^T\delta\left(\frac{\partial T}{\partial z}\right)\right]\mathrm{d}V + \int_{V_c}\left[k_c\left(\frac{\partial T}{\partial x}\right)^T\delta\left(\frac{\partial T}{\partial x}\right)+k_c\left(\frac{\partial T}{\partial y}\right)^T\delta\left(\frac{\partial T}{\partial y}\right)+k_c\left(\frac{\partial T}{\partial z}\right)^T\delta\left(\frac{\partial T}{\partial z}\right)\right]\mathrm{d}V + \int_{V_m}\rho_m c_m\dot{T}\delta T\,\mathrm{d}V+\int_{V_c}\rho_c c_c\dot{T}\delta T\,\mathrm{d}V+\tilde{\alpha}\int_{S_1}(T-T_1)\delta T\,\mathrm{d}S+\tilde{\alpha}\int_{S_2}(T-T_2)\delta T\,\mathrm{d}S \tag{9}$$

Setting d$I^*(T)$ = 0 for arbitrary δT in eq. (9), results in the following set of linear equations

$$KT + M\dot{T} = f \tag{10a}$$

where

$$K_{ij}=\int_{V_m}\begin{Bmatrix}\Phi_{ix}\\ \Phi_{iy}\\ \Phi_{iz}\end{Bmatrix}^T\begin{bmatrix}k_m & 0 & 0\\ 0 & k_m & 0\\ 0 & 0 & k_m\end{bmatrix}\begin{Bmatrix}\Phi_{jx}\\ \Phi_{jy}\\ \Phi_{jz}\end{Bmatrix}\mathrm{d}V+\int_{V_c}\begin{Bmatrix}\Phi_{ix}\\ \Phi_{iy}\\ \Phi_{iz}\end{Bmatrix}^T\begin{bmatrix}k_c & 0 & 0\\ 0 & k_c & 0\\ 0 & 0 & k_c\end{bmatrix}\begin{Bmatrix}\Phi_{jx}\\ \Phi_{jy}\\ \Phi_{jz}\end{Bmatrix}\mathrm{d}V + \int_{S_1}\tilde{\alpha}\Phi_i^T\Phi_j\,\mathrm{d}S+\int_{S_1}\tilde{\alpha}\Phi_i^T\Phi_j\,\mathrm{d}S \tag{10b}$$

$$M_{ij}=\int_{V_m}\rho_m c_m\Phi_i^T\Phi_j\,\mathrm{d}V+\int_{V_c}\rho_c c_c\Phi_i^T\Phi_j\,\mathrm{d}V \tag{10c}$$

$$\mathrm{f}_i \quad \tilde{\alpha} T_1 \Phi_i \,\mathrm{d}S_{S_1} \quad \tilde{\alpha} T_2 \Phi_i \,\mathrm{d}S_{S_2} \tag{10d}$$

Using α-family of approximation scheme for time discretization, the eq. (10a) is modified as:

$$(\tilde{K} \quad M) T^{\tilde{n} \;\; 1} \quad R^{\tilde{n}} \tag{11a}$$

where

$$R^{\tilde{n}} \quad [M \quad (1 \quad \alpha)\Delta t K] T^{\tilde{n}} \quad \Delta t f \text{ and } \tilde{K} \quad \alpha \Delta t K \tag{11c}$$

Assuming material properties as homogeneous and independent of temperature, the thermal conductivities of the composite in longitudinal direction of nanotube has been evaluated as:

$$k_\mathrm{e} \quad \frac{q_\mathrm{avg} L_\mathrm{b}}{\Delta T} \tag{12}$$

where k_e denote the equivalent thermal conductivities of the composite in longitudinal direction, L_b is the length, q_avg is the average normal heat flux, ΔT is the temperature difference between two opposite ends, S_1 and S_2 (eqs. 8, 9, 10b, and 10d) indicate the left and right surfaces of the square RVE on which temperature is applied.

Numerical results and discussion

For transient simulations, a model CNT-composite problem has been solved by EFG method. Penalty approach has been used to enforce boundary conditions *i. e.* constant temperatures at two square surfaces of RVE. The simulations have been carried out for two different values of nanotube length. Three point Gauss quadrature scheme has been used for the numerical integration of Galerkin weak form. Both nanotube and matrix domains have been discretized using non-uniform nodal distribution schemes. The time discretization has been performed by both backward difference and Galerkin approaches. The following data has been used for nanotube [12, 16] and PEEK polymer matrix [17] along with other dimensions: $k_\mathrm{m} = 0.25$ W/mK, $\rho_\mathrm{m} = 1320$ kg/m^3, $c_\mathrm{m} = 335$ J/kgK, $k_\mathrm{c} = 3000$ W/mK, $\rho_\mathrm{c} = 2600$ kg/m^3, $c_\mathrm{c} = 500$ J/kgK, $L_\mathrm{b} = 10$ μm, $L_\mathrm{c} = 6$ and 8 μm, $H_\mathrm{b} = W_\mathrm{b} = 40$ nm, $\mathrm{r_o} = 10$ nm, $T_1 = 300$ K, and $T_2 = 100$ K.

The results presented in fig. 2 have been obtained for two values of nanotube length *i. e.* $L_\mathrm{c} = 6$ and 8 μm at the location $y = W_\mathrm{b}/2$, $z = H_\mathrm{b}$, and it shows a transient temperature distribution at

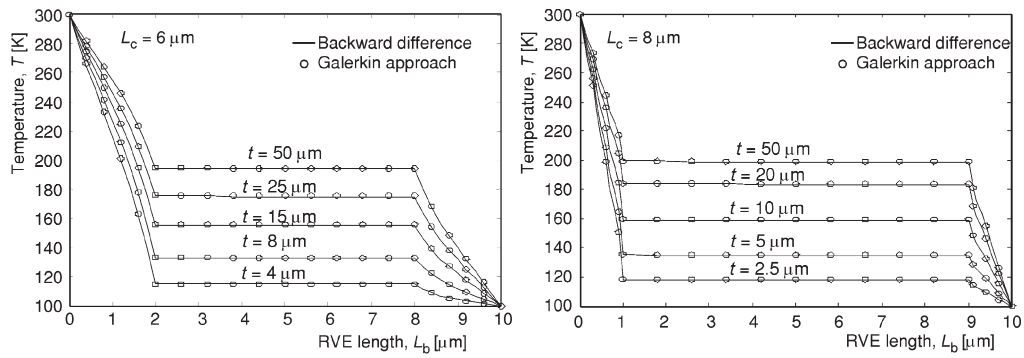

Figure 2. Transient temperature distribution at $y = W_\mathrm{b}/2$, $z = H_\mathrm{b}$ for various values of time

$t = 4$, 8, 15, 25, and 50 μs for $L_c = 6$ μm and at $t = 2.5$, 5, 10, 20, and 50 μs for $L_c = 8$ μm. The similar types of results have been presented in fig. 3 at another location ($y = W_b/2$, $z = 0.8\ H_b$). Figure 4 shows a transient temperature distribution on the CNT surface for $L_c = 6$ and 8 μm. The results presented in fig. 5 have been obtained at location $x = L_1/2 + L_c$, $y = W_b/2$, and it shows the temperature

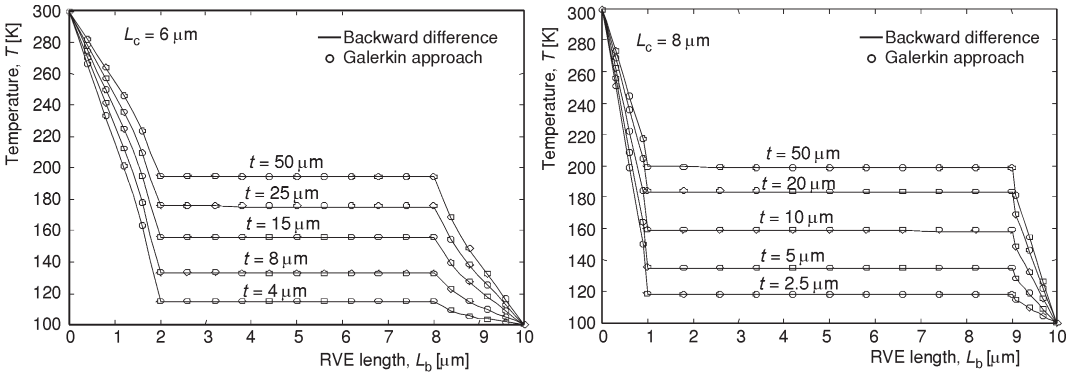

Figure 3. Transient temperature distribution at $y = W_b/2$, $z = 0.8\ H_b$ for various values of time

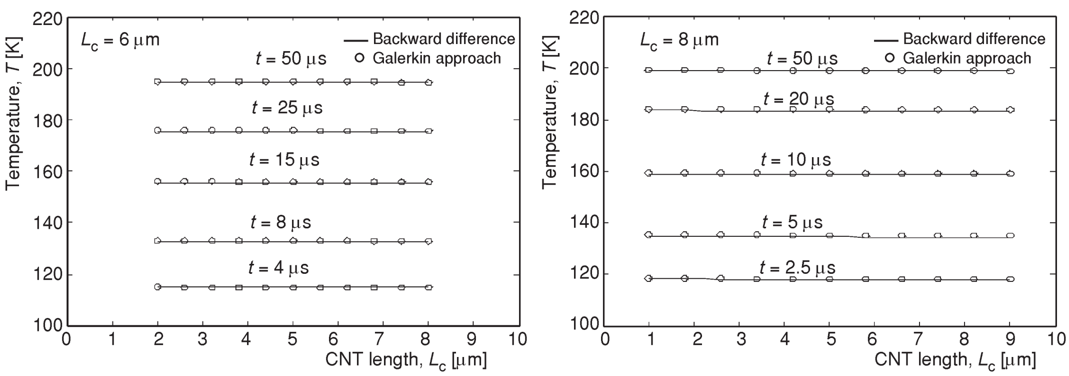

Figure 4. Transient temperature distribution at CNT surface for various values of time

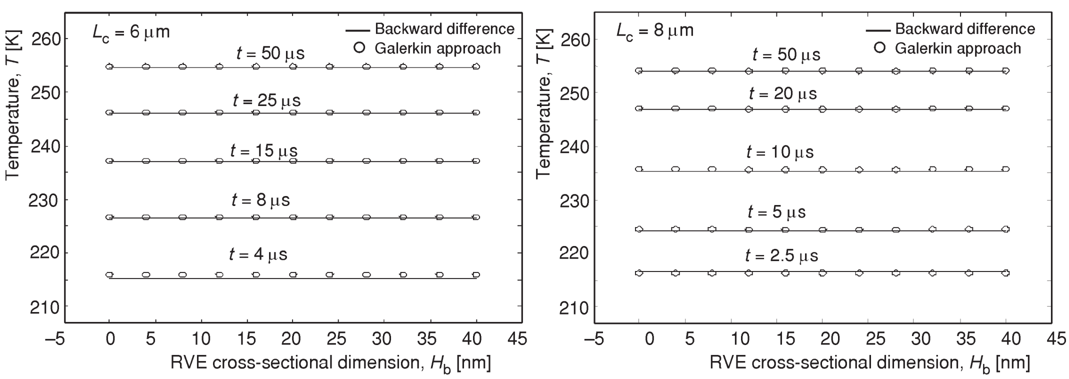

Figure 5. Transient temperature distribution at $x = L_1/2$, $y = W_b/2$ for various values of time

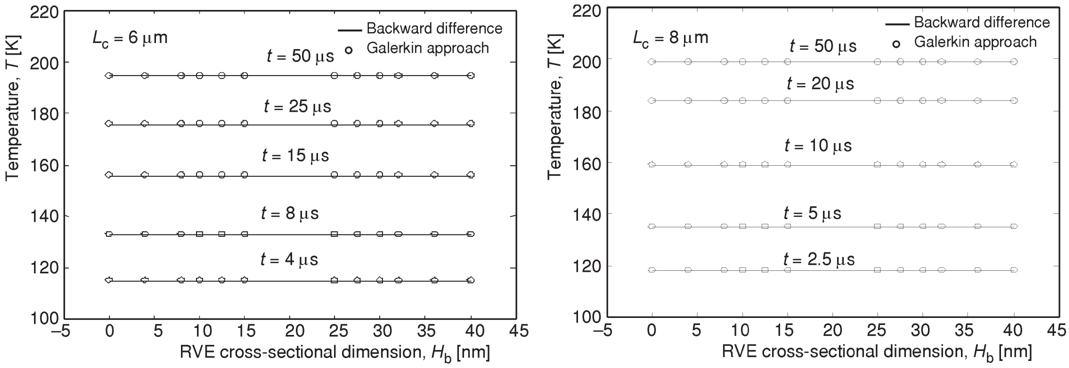

Figure 6. Transient temperature distribution at $x = L_1$, $y = W_b/2$ for various values of time

distribution at $t = 4$, 8, 15, 25, and 50 μs for $L_c = 6$ μm, and at $t = 2.5$, 5, 10, 20, and 50 μs for $L_c = 8$ μm. The similar types of results have been presented in fig. 6 at the location ($x = L_1$, $y = W_b/2$), in fig. 7 at the location $x = L_1 + L_c/2$, $y = W_b/2$, in fig. 8 at the location $x = L_1 + L_c$, $y = W_b/2$, and in fig. 9 at the location ($x = L_b - L_1/2$, $y = W_b/2$). Figure 10 presents the variation of av-

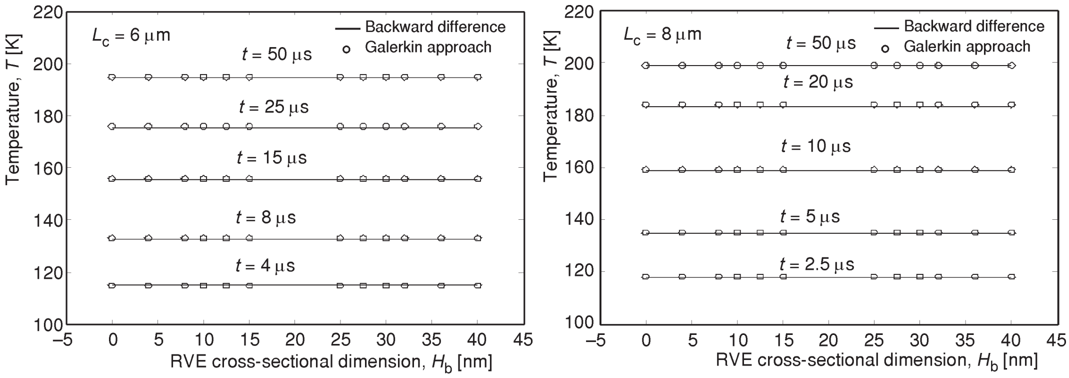

Figure 7. Transient temperature distribution at $x = L_1 + L_c/2$, $y = W_b/2$ for various values of time

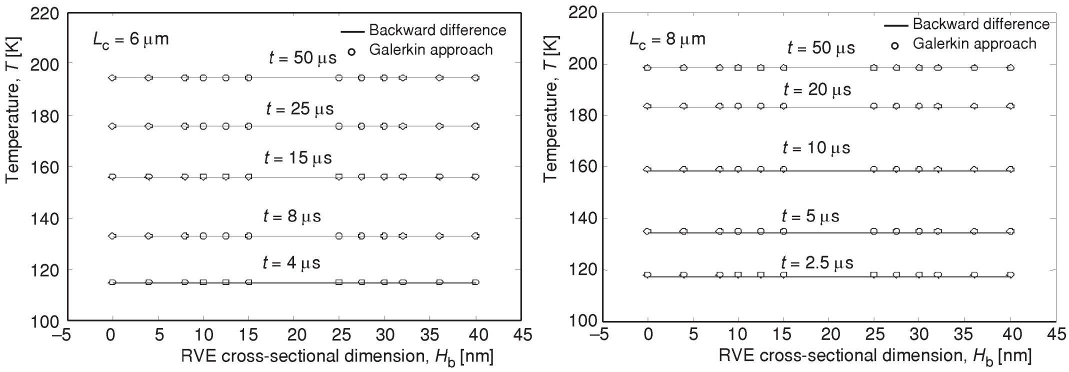

Figure 8. Transient temperature distribution at $x = L_1 + L_c$, $y = W_b/2$ for various values of time

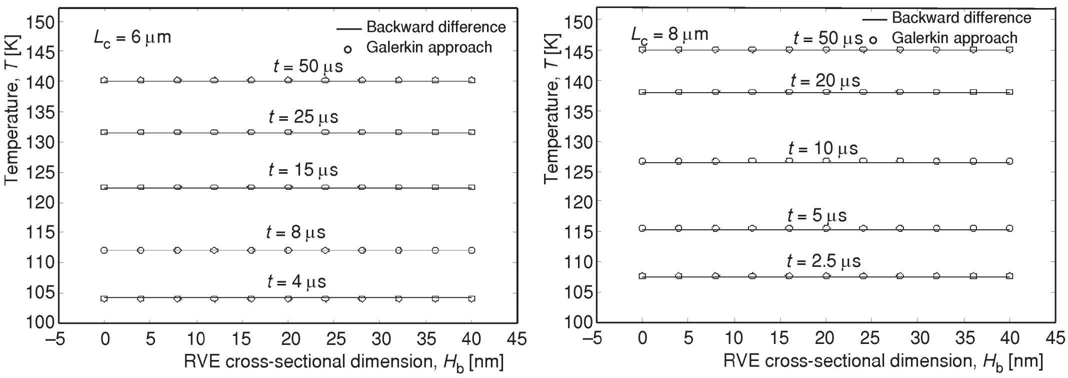

Figure 9. Transient temperature distribution at $x = L_b - L_1/2$, $y = W_b/2$ for various values of time

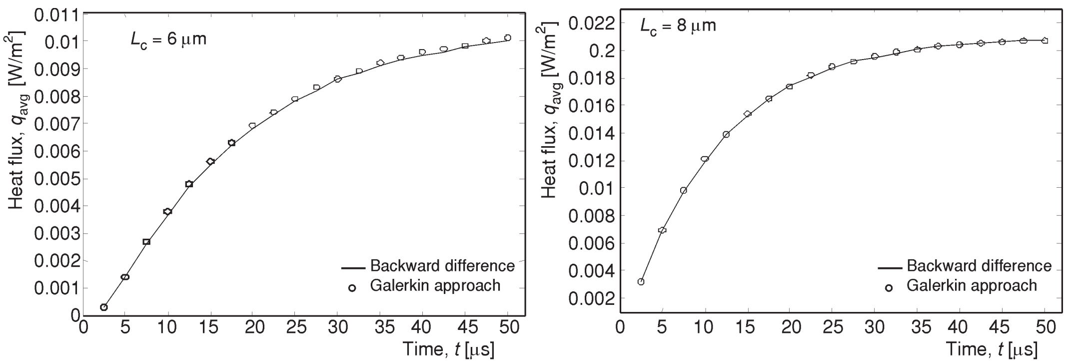

Figure 10. The variation of average heat flux with time on right RVE surface

erage heat flux obtained by backward difference and Galerkin approaches with time (t) for $L_c = 6$ and 8 μm, whereas fig. 11 shows the variation of k_e/k_m obtained by backward difference and Galerkin approaches with time for the same values of L_c. From the results presented in figs. 2-11, it can be concluded that the results obtained by backward different scheme are almost same as those obtained by Galerkin approach.

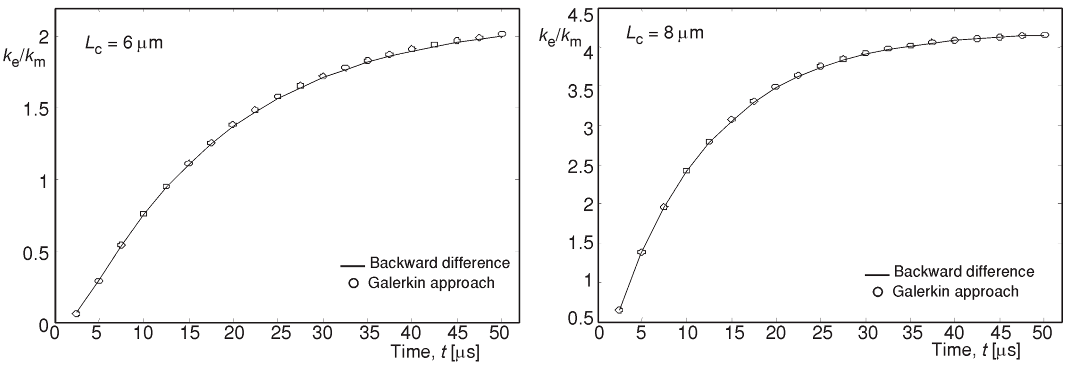

Figure 11. The variation of equivalent thermal conductivity of the composite with time

Conclusions

In this paper, transient thermal analysis of carbon nanotube composites was performed via meshless element free Galerkin method. A three-dimensional representative volume element containing single nanotube was taken as model for the transient thermal simulation. Essential boundary conditions were enforced by penalty approach. Simulations were carried out using continuum mechanics approach for two different values of nanotube length. Backward difference and Galerkin approaches were utilized for the approximation of time. The results obtained by backward difference method were compared with those obtained by Galerkin approach, and were found in good agreement with each other. This work can be extended further for the transient thermal analysis of CNT-composites containing carbon nanotubes randomly distributed in polymer matrix. Moreover, this analysis can be very useful in the preparation and selection of composite materials for electrical and electronic devices.

Acknowledgment

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Nomenclature

c_c – specific heat of nanotube, [$Jkg^{-1}K^{-1}$]
c_m – specific heat of polymer matrix (PEEK), [$Jkg^{-1}K^{-1}$]
k_c – thermal conductivity of nanotube, [$Wm^{-1}K^{-1}$]
k_e – equivalent thermal conductivity of composite, [$Wm^{-1}K^{-1}$]
k_m – thermal conductivities of polymer matrix (PEEK), [$Wm^{-1}K^{-1}$]
L_b – length of square RVE, [nm]
L_c – nanotube length, [nm]
m' – number of terms in basis function
n – number of nodes in the domain of influence
$\tilde{n}$ – times step number
$p_j(x)$ – monomial basis function
q_{avg} – normal heat flux, [Wm^{-2}]
r_o – nanotube, [nm]
$T^h(x)$ – MLS approximation function for temperature
V_c – nanotube domain
V_m – matrix domain
w – weight function used in MLS approximation
$\tilde{w}$ – weighting function used in weighted integral form

Greek letters

α – parameter used in time integration schemes
$\tilde{\alpha}$ – penalty parameter
ρ_c – density of nanotube, [kgm^{-3}]
ρ_m – density of polymer matrix (PEEK), – [kgm^{-3}]
$\Phi_i(x)$ – shape function

Subscripts

c – nanotube
m – matrix

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