Evaluation of effective thermal conductivity of CNT-based nano-composites by element free Galerkin method

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Abstract

Purpose – The purpose of this paper is to evaluate the thermal properties of carbon nanotube composites via meshless element free Galerkin (EFG) method.

Design/methodology/approach – The EFG method is based on moving least square approximation, which is constructed by three components: a weight function associated with each node, a basis function and a set of non-constant coefficients. In principle, EFG method is almost identical to finite element method. The EFG method does not require elements for the interpolation (or approximation) of field variable, but only requires a set of nodes for the construction of approximation function.

Findings – The equivalent thermal conductivity of the composite has been calculated, and plotted against nanotube length, nanotube radius, RVE length, and RVE radius. Temperature distribution has been obtained and plotted with RVE length. An approximate numerical formula is proposed to calculate the equivalent thermal conductivity of CNT-composites. Present computations show that the addition of 6.2 per cent (by volume) of CNT in polymer matrix increases the thermal conductivity of the composite by 42 per cent, whereas 16.1 per cent of CNT addition increases the thermal conductivity of the composite by 352 per cent.

Research limitations/implications – An ideal model, i.e. representative volume element containing single CNT has been taken to evaluate the thermal properties of CNT-composites.

Practical implications – A simplified approach based on EFG method has been developed to evaluate the overall thermal conductivity of the CNT-composites.

Originality/value – Continuum mechanics-based mesh-free EFG method has been successfully implemented for the thermal analysis of CNT-composites.

Keywords Carbon, Composite materials, Thermal conductivity, Galerkin method

Paper type Research paper

Nomenclature

k_m = thermal conductivity of matrix, W/m-K

k_e = equivalent thermal conductivity of composite, W/m-K

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L	= length of cylindrical RVE, nm	w	= weight function used in MLS approximation
L_c	= CNT length, nm	$\bar{w}$	= weighting function used in weighted residual form
m	= number of terms in basis	α	= penalty parameter
n	= number of nodes in the domain of influence	Γ	= boundary of the computational domain
$p_j(\mathbf{r})$	= monomial basis function	Γ_3	= CNT surface
q	= heat flux, W/m^2	Ω	= two-dimensional domain
r_o	= outer radius of CNT, nm	$\Phi_I(\mathbf{r})$	= shape function
R_o	= radius of cylindrical RVE, nm		
T_c	= constant temperature at CNT surface, K		
$T^h(\mathbf{r})$	= MLS approximation function for temperature		

1. Introduction

The need of reducing the size and weight of the electronic devices has attracted the interest of many researchers towards the field of nanotechnology. Among various MEMS/NEMS applications, carbon nanotubes (CNTs) have got a unique position due to their light weight, high stability, special electronic structure, and excellent mechanical, electrical and thermal properties. These properties make the CNTs an ideal reinforcing material for future composites. The mechanical properties of CNTs have been studied by many researchers through experimental work (Bower *et al.*, 1999; Qian *et al.*, 2000; Schadler *et al.*, 1998; Wagner *et al.*, 1998) and numerical simulations (Srivastava *et al.*, 2001; Liu and Chen, 2003a, b; Chen and Liu, 2004; Liu *et al.*, 2005a, b). It has been found that by addition of only 1 per cent (by weight) of CNTs in a matrix, the stiffness of the resulting composite increases by 36-42 per cent and tensile strength by 25 per cent (Chen and Liu, 2004). These studies shows, that the CNT-based composites have capability of providing a new class of materials.

It is now widely accepted that the thermal behavior of nano-materials becomes increasingly important with the reduction of device size, since it plays an important role in the stability and performance of the device. So far, not much work has been done on the thermal behavior of CNT-based composites. Recently, few simulations were carried out to evaluate the thermal properties of CNT composites. Song and Youn (2006) applied the control volume finite element method to evaluate the effective thermal conductivity of carbon nanotube-polymer (epoxy) composites. Nishimura and Liu (2004) used the boundary integral equation formulation for the thermal analysis of CNT-based nano-composites. They solved the heat conduction problems in 2D infinite domain embedded with many rigid inclusions with the help of a fast multipole boundary element method. Zhang *et al.* (2004a, b) and Tanaka *et al.* (2003) used the meshless hybrid boundary node method (hybrid BNM) for the heat conduction analysis of CNT-based nano-composites. They used multi-domain and simplified approaches coupled with fast multipole method to solve large-scale problems. In their study, they found that the addition of 7.2 per cent (by volume) of CNTs in the polymer matrix increases thermal conductivity of the composite by 49 per cent.

Till date, mostly boundary type methods such as BEM and hybrid BNM were used to predict the thermal behavior of CNT-based composites, but these methods do not have symmetry, bandedness and sparseness properties in their solution matrix; therefore, the solution of large-scale problems is relatively difficult and expensive task.

Although, fast multiple method (FMM) can alleviate this difficulty to some extent, but the implementation of FMM is still an extremely complicated and burdensome task. On the other hand, domain type element-free Galerkin (EFG) method possesses all these properties and can be extended to deal with large-scale problems. Therefore, in the present work, meshless EFG method has been used as an initial step to evaluate the thermal properties of CNT-based nano-composites. Continuum mechanics approach has been used to evaluate the thermal properties of nano-composites. A sensitivity analysis of RVE as well as nanotube dimensions has been carried out in detail. The equivalent thermal conductivity has been plotted as function of nanotube length, nanotube radius, RVE length and RVE radius. Temperature profile has been obtained at two critical locations of RVE. An approximate numerical formula is proposed to evaluate the equivalent thermal conductivity of nano-composites. The results obtained by EFG method have been found in good agreement with those obtained by hybrid boundary node method.

2. The element-free Galerkin method

The discretization of the governing equations by EFG method requires moving least square (MLS) approximants, which are made up of three components: a weight function associated with each node, a basis function and a set of non-constant coefficients. Using MLS approximation, the unknown temperature function $T(\mathbf{r})$ is approximated as $T^h(\mathbf{r})$ (Singh *et al.*, 2004):

$$T^h(\mathbf{r}) = \sum_{j=1}^{m} p_j(\mathbf{r}) a_j(\mathbf{r}) = \mathbf{p}^T(\mathbf{r})\mathbf{a}(\mathbf{r}) \tag{1}$$

where $\mathbf{r}^T = [\,r \quad z\,]$, $\mathbf{p}^T(\mathbf{r}) = [\,1 \quad r \quad z\,]$, $m = 3$ and $\mathbf{a}^T(\mathbf{r}) = [\,a_1(\mathbf{r}), \quad a_2(\mathbf{r}), \quad a_3(\mathbf{r})\,]$

The unknown coefficients $\mathbf{a}(\mathbf{r})$ at any given point are determined by minimizing the functional J:

$$J = \sum_{I=1}^{n} w(\mathbf{r} - \mathbf{r}_I)[\mathbf{p}^T(\mathbf{r}_I)\mathbf{a}(\mathbf{r}) - T_I]^2 \tag{2}$$

where n is the number of nodes in the neighborhood of $\mathbf{r}$ for which the weight function $w(\mathbf{r} - \mathbf{r}_I) \neq 0$, and T_I is the nodal parameter at $\mathbf{r} = \mathbf{r}_I$. The stationary value of J in equation (2) w.r.t. $\mathbf{a}(\mathbf{r})$ leads to following system of linear equations:

$$\mathbf{a}(\mathbf{r}) = \mathbf{A}^{-1}(\mathbf{r})\mathbf{B}(\mathbf{r})\mathbf{T} \tag{3}$$

where:

$$\mathbf{A}(\mathbf{x}) = \sum_{I=1}^{n} w(\mathbf{x} - \mathbf{x}_I)\mathbf{p}(\mathbf{x}_I)\mathbf{p}^T(\mathbf{x}_I), \tag{4}$$

$$\mathbf{B}(\mathbf{x}) = \{w(\mathbf{x} - \mathbf{x}_1)\mathbf{p}(\mathbf{x}_1), w(\mathbf{x} - \mathbf{x}_2)\mathbf{p}(\mathbf{x}_2), \ldots, w(\mathbf{x} - \mathbf{x}_n)\mathbf{p}(\mathbf{x}_n)\}, \tag{5}$$

$$\mathbf{T}^T = [T_1, T_2, T_3, \ldots, T_n]. \tag{6}$$

By substituting equation (3) in equation (1), the MLS approximants can be obtained as:

$$
\begin{aligned}
T^h(\mathbf{r}) &= \mathbf{p}^T(\mathbf{r})\mathbf{A}^{-1}(\mathbf{r})\mathbf{B}(\mathbf{r})\mathbf{T} \\
&= \sum_{I=1}^{n}\sum_{j=1}^{m} p_j(\mathbf{r})(\mathbf{A}^{-1}(\mathbf{r})\mathbf{B}(\mathbf{r}))_{jI} \\
&= \sum_{I=1}^{n} \Phi_I(\mathbf{r})T_I = \mathbf{\Phi}(\mathbf{r})\mathbf{T}
\end{aligned}
\tag{7}
$$

where T_I are the nodal parameters and $\Phi_I(\mathbf{r})$ is the shape function, which is defined as:

$$
\Phi_I(\mathbf{r}) = \sum_{j=1}^{m} p_j(\mathbf{r})(\mathbf{A}^{-1}(\mathbf{r})\mathbf{B}(\mathbf{r}))_{jI} = \mathbf{p}^T\mathbf{A}^{-1}\mathbf{B}_I. \tag{8}
$$

Exponential weight function (Singh *et al.*, 2004) has been used in this work, which is given as:

$$
w(s) = \begin{Bmatrix} C^{-s} & 0 \leq s \leq 1 \\ 0 & s > 1 \end{Bmatrix} \tag{9}
$$

where constant C should be taken in the range of $1,000 \leq C \leq 5,000$ to get smooth shape function, $s = \|\mathbf{r} - \mathbf{r}_I\|/\mathrm{d}_{mI}$ is the normalized radius, $\mathrm{d}_{mI} = \mathrm{d}_{\max} c_I$ with $c_I = \max_J |\mathbf{r}_I - \mathbf{r}_J|$ and $\mathrm{d}_{\max}$ = scaling parameter. Please refer article by Belytschko *et al.* (1994) for full details of EFG method.

3. Numerical formulation

A real CNT composite may have CNTs of different shapes and sizes such as straight or curved, short or long, aligned or arbitrarily oriented, and randomly distributed in polymer matrix. The properties evaluation of these composites is quite necessary for applications point of view. But the present analysis is limited to RVE containing single CNT only.

CNTs are having very high value of thermal conductivity as compared to polymers. This unusually high value of thermal conductivity makes CNTs to behave as a superconductor inside polymer matrix. It has been demonstrated by numerical simulations that CNTs behave as superconductor inside polymer (Zhang *et al.*, 2004a, b), and a nearly constant temperature has been found on surface of CNT.

In the present work, CNT is assumed at an unknown constant temperature, therefore only matrix domain has been modeled. A model problem (Figure 1) containing single CNT inside cylindrical RVE has been considered. CNT has been placed symmetrically at the center of RVE such that the axis of RVE coincides with the axis of nanotube. Two different values of temperatures have been applied at two ends of RVE, and outer cylindrical surface has been kept insulated. This problem has been solved by treating it an axisymmetric heat transfer problem governed by Laplace equation. The steady sate heat conduction equation in cylindrical coordinate system with thermal properties independent of temperature is given as:

$$
\frac{1}{r}\frac{\partial}{\partial r}\left(k_{\mathrm{m}} r \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k_{\mathrm{m}} \frac{\partial T}{\partial z}\right) = 0 \tag{10a}
$$

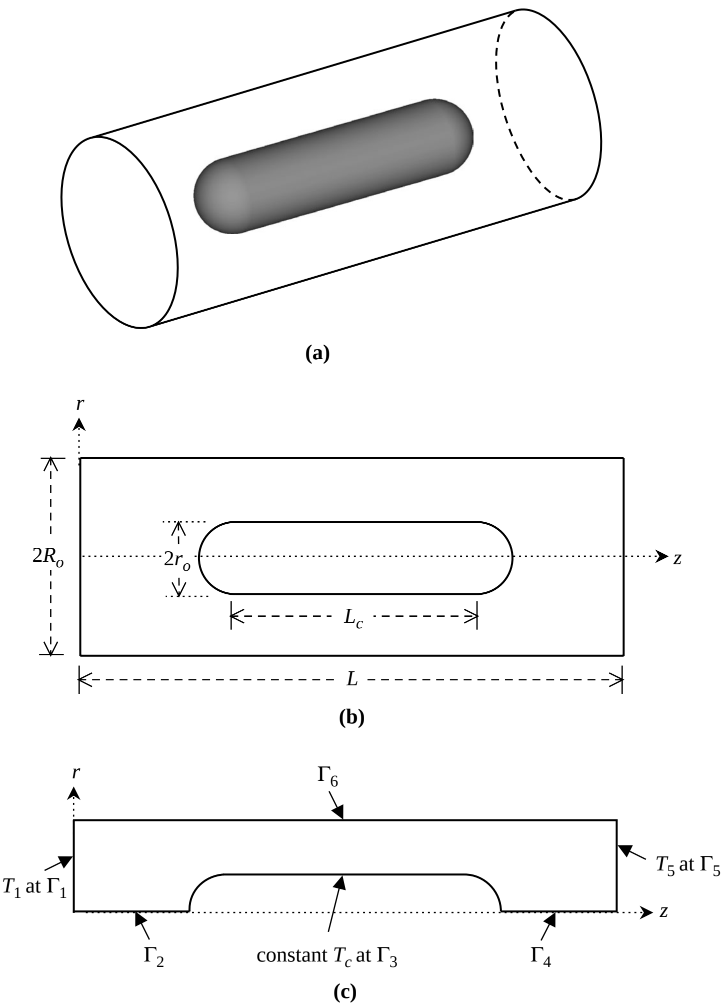

Figure 1.
Model for CNT problem: (a) nanoscale cylindrical representative volume element containing single nanotube; (b) dimensions of the model; (c) 2-D model with boundary conditions

with the following essential boundary conditions:

$$\text{at } z = 0, \quad T = T_1 \tag{10b}$$

$$\text{at } z = L, \quad T = T_5. \tag{10c}$$

The weighted integral form of equation (10a) is given as:

$$\int_\Omega \bar{w}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(k_\mathrm{m} r\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k_\mathrm{m}\frac{\partial T}{\partial z}\right)\right]2\pi r \mathrm{d}r\mathrm{d}z = 0. \tag{11}$$

From equation (11), the functional $I(T)$ can be obtained as:

$$I(T) = 2\pi \int_{\Omega} \frac{1}{2} k_{\rm m} \left[\left(\frac{\partial T}{\partial r} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] r {\rm d}r {\rm d}z. \tag{12}$$

Since, CNT surface is assumed to have an unknown constant temperature, therefore, enforcing essential boundary conditions using penalty method, the functional $I^*(T)$ is obtained as:

$$\begin{aligned} I^*(T) = 2\pi \int_{\Omega} \frac{1}{2} k_{\rm m} \left[\left(\frac{\partial T}{\partial r} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] r {\rm d}r {\rm d}z + \frac{\alpha}{2} \int_{\Gamma_1} (T - T_1)^2 {\rm d}\Gamma \\ + \frac{\alpha}{2} \int_{\Gamma_3} (T - T_{\rm c})^2 {\rm d}\Gamma + \frac{\alpha}{2} \int_{\Gamma_5} (T - T_5)^2 {\rm d}\Gamma. \end{aligned} \tag{13}$$

Taking variation, i.e. $\delta I^*(T)$ of equation (13), it reduces to:

$$\begin{aligned} \delta I^*(T) = 2\pi \int_{\Omega} k_{\rm m} \left[\left(\frac{\partial T}{\partial r} \right)^T \delta \left(\frac{\partial T}{\partial r} \right) + \left(\frac{\partial T}{\partial z} \right)^T \delta \left(\frac{\partial T}{\partial z} \right) \right] r {\rm d}r {\rm d}z \\ + \alpha \int_{\Gamma_1} (T - T_1) \delta T {\rm d}\Gamma + \alpha \int_{\Gamma_3} (T - T_{\rm c}) \delta T {\rm d}\Gamma \\ + \alpha \int_{\Gamma_5} (T - T_5) \delta T {\rm d}\Gamma. \end{aligned} \tag{14}$$

Since, $\delta I^*(T) = 0$ and δT are arbitrary in equation (14), a following set of equations is obtained using equation (7):

$$[\mathbf{K}]\{\mathbf{T}\} = \{\mathbf{f}\} \tag{15a}$$

where:

$$\begin{aligned} K_{IJ} = 2\pi \int_{\Omega} \begin{bmatrix} \Phi_{I,r} \\ \Phi_{I,z} \end{bmatrix}^T \begin{bmatrix} k_{\rm m} & 0 \\ 0 & k_{\rm m} \end{bmatrix} \begin{bmatrix} \Phi_{I,r} \\ \Phi_{I,z} \end{bmatrix} r {\rm d}r {\rm d}z \\ + \alpha \int_{\Gamma_1} \Phi_I \Phi_J {\rm d}\Gamma + \alpha \int_{\Gamma_3} \Phi_I \Phi_J {\rm d}\Gamma + \alpha \int_{\Gamma_5} \Phi_I \Phi_J {\rm d}\Gamma \end{aligned} \tag{15b}$$

$$f_I = \alpha \int_{\Gamma_1} T_1 \Phi_I {\rm d}\Gamma + \alpha \int_{\Gamma_3} T_{\rm c} \Phi_I {\rm d}\Gamma + \alpha \int_{\Gamma_5} T_5 \Phi_I {\rm d}\Gamma. \tag{15c}$$

The equation (15a) is further written as:

$$\begin{bmatrix} \mathbf{K}_{pp} & \mathbf{K}_{pq} \\ \mathbf{K}_{qp} & \mathbf{K}_{qq} \end{bmatrix} \begin{Bmatrix} \mathbf{T}_p \\ \mathbf{T}_q \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_p \\ \mathbf{f}'_q T_{\rm c} \end{Bmatrix} \tag{16a}$$

where:

$$(f_P)_I = \alpha \int_{\Gamma_1} T_L \Phi_I \mathrm{d}\Gamma + \alpha \int_{\Gamma_5} T_R \Phi_I \mathrm{d}\Gamma \tag{16b}$$

$$(f'_q)_I = \alpha \int_{\Gamma_3} \Phi_I \mathrm{d}\Gamma \tag{16c}$$

$$\begin{bmatrix} \mathbf{K}_{pp} & \mathbf{K}_{pq} \\ \mathbf{K}_{qp} & \mathbf{K}_{qq} \end{bmatrix} = [\mathbf{K}]. \tag{16d}$$

$\mathbf{T}_q$ and $\mathbf{T}_p$ are the values of temperature degree of freedom on CNT surface and rest of the domain, respectively, and T_c is the unknown constant temperature on the CNT surface, which requires one additional equation to solve the system of equations. This additional equation can be obtained by using law of conservation of energy at the CNT surface. In other words, net rate of thermal energy flowing through CNT surface is zero, i.e. $\int_{\Gamma_3} q \mathrm{d}\Gamma = 0$. Substituting $\int_{\Gamma_3} q \mathrm{d}\Gamma = 0$ in equation (16a), it takes the following form:

$$\begin{bmatrix} \mathbf{K}_{pp} & \mathbf{K}_{pq} & 0 \\ \mathbf{K}_{qp} & \mathbf{K}_{qq} & -\mathbf{f}'_q \\ 0 & \mathbf{f}''_q & 0 \end{bmatrix} \begin{Bmatrix} \mathbf{T}_p \\ \mathbf{T}_q \\ T_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_p \\ 0 \\ 0 \end{Bmatrix} \tag{17}$$

where $(f''_q)_I = \int_{\Gamma_3} \mathrm{d}\Phi/\mathrm{d}n' \mathrm{d}\Gamma$ with n' is the outward normal to the surface.

4. Numerical results and discussion

In this section, a model problem (Figure 1) has been solved to evaluate the thermal conductivity of the composite using EFG method. The computational model along with boundary conditions is shown in Figure 1(c). The data used for the model problem is given in Table I. Penalty approach has been used to enforce the essential boundary conditions. The EFG results have been obtained using uniform nodal distribution scheme for 4,941 nodes. Assuming material properties as homogeneous, isotropic and independent of temperature, the equivalent thermal conductivity of the composite can be evaluated as:

Parameters	Value of parameters
Total length of RVE (L)	100 nm
Nanotube length (L_c)	50 nm
RVE radius (R_o)	11.28 nm
Carbon nanotube outer radius (r_o)	5 nm
Thermal conductivity of polycarbonate matrix (k_m)	0.19 W/m-K
Temperature at $\Gamma_1(T_1)$	300 K
Temperature at $\Gamma_5(T_5)$	200 K
Penalty parameter (α)	10^4

Table I. Data for CNT based composite problem

$$k_e = -\frac{qL}{\Delta T} \tag{18}$$

where k_e denotes the equivalent thermal conductivity of the composite, L is the length of RVE, q is normal heat flux density, and ΔT is the temperature difference between two ends of RVE.

In the present simulation, the percentage volume fraction (Zhang *et al.*, 2004a, b) has been calculated by the following expression:

$$v = \left(\frac{V_c}{V_c + V_m}\right) \times 100 \tag{19}$$

where v is the percentage volume fraction of CNT in composite, V_c is the volume of CNT including cavity and V_m is the volume of polymer (polycarbonate) matrix.

Zhang *et al.* (2004a) proposed an approximate formula to evaluate the equivalent thermal conductivity of CNT-based composites:

$$k_e = k_m\left(\frac{L}{L - L_c - 0.4r_o}\right). \tag{20}$$

In the present work, authors have presented a more accurate, approximate formula to evaluate the equivalent thermal conductivity of the composite:

$$k_e = k_m\left(\frac{L}{0.95L + 1.45R_o - L_c - 2.8r_o}\right) \tag{21}$$

where k_e = equivalent thermal conductivity of the nano-composite, k_m = thermal conductivity of the polymer matrix, L = RVE length, R_o = radius of cylindrical RVE, L_c = nanatube length and r_o = nanotube radius.

In the following sub-sections, temperature distribution with RVE length and variation of equivalent thermal conductivity with nanotube length, nanotube radius, RVE length and RVE radius has been presented, and discussed in detail.

4.1 Temperature distribution in cylindrical RVE

The values of temperature have been obtained for the data presented in Table I and its distribution with RVE length is shown in Figure 2 at two typical locations, i.e. $r = 5.314$ and 6.256 nm. From the results shown in Figure 2, it can be observed that the temperature first decreases rapidly from left cylindrical edge (300 K) to the left end of CNT (250 K) after that it remains almost constant (250 K) along CNT length near the CNT surface, then it again start decreasing from right end of CNT (250 K) to 200 K. These observations show that almost entire heat flux passes through nanotube in the composite. The results obtained by EFG method have also been compared with those obtained by hybrid boundary node method [13], and were found in good agreement with hybrid BNM.

4.2 Effect of CNT length (L_c) on thermal conductivity

This sub-section describes the effect of CNT length on the equivalent thermal conductivity of the composite. The different parameters required for this analysis are given in Table I. Various values of CNT length, i.e. from 25 to 75 nm have been taken to

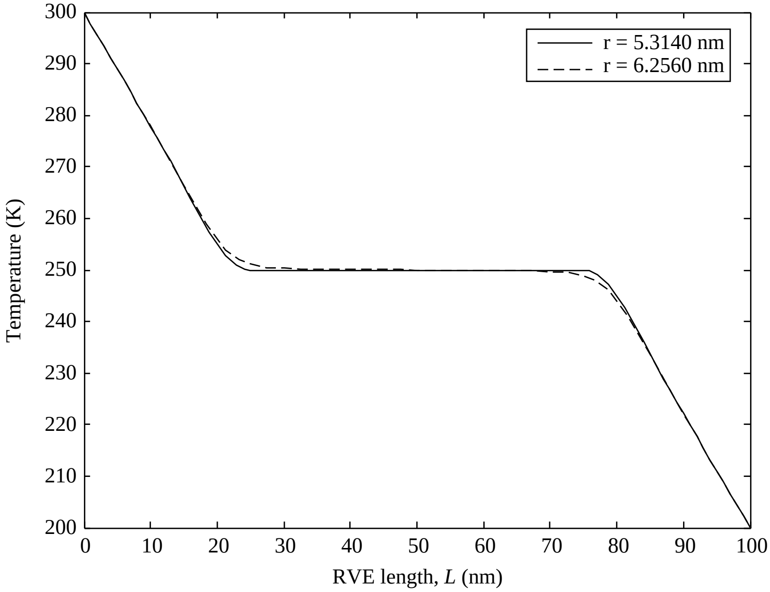

Figure 2.
Variation of temperature with RVE length

study the effect of CNT length on equivalent thermal conductivity of the composite. Figure 3 shows the variation of equivalent thermal conductivity of the composite with CNT length. The addition of 6.2 per cent (equivalent to $L_c = 25\,\text{nm}$) of CNT by volume increases the equivalent thermal conductivity of the composite by 1.42 times that of polymer matrix, whereas 16.1 per cent (equivalent to $L_c = 75\,\text{nm}$) of CNT addition

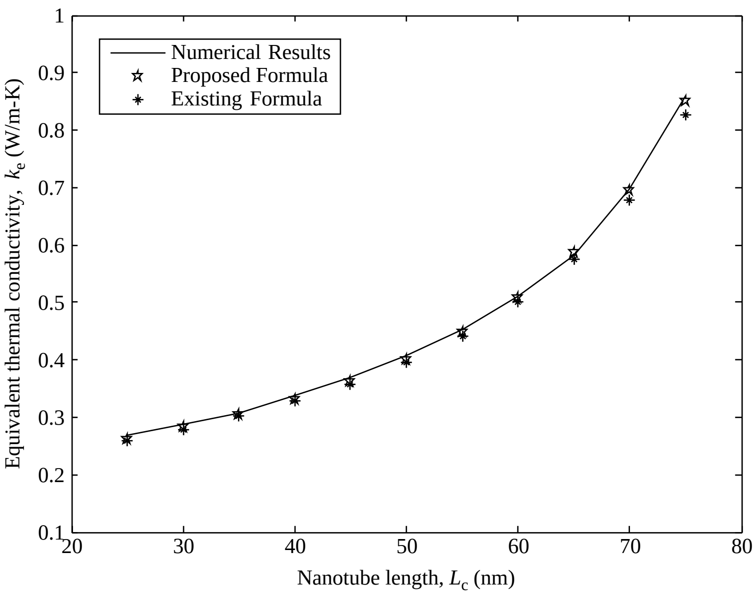

Figure 3.
Variation of equivalent thermal conductivity with CNT length

increases the equivalent thermal conductivity of the composite by 4.53 times that of polymer matrix. The results obtained by numerical method and proposed formula have been compared with those obtained by existing formula, and have been found in good conformity with each other.

4.3 Effect of CNT radius (r_o) on thermal conductivity

In this sub-section, two different values of nanotube length, i.e. $L_c = 40$ and 50 nm have been chosen to study the effect of nanotube radius on the equivalent thermal conductivity of the composite. The equivalent thermal conductivity of the composite obtained by numerical method, proposed formula and existing formula for various values of CNT radius is shown in Figure 4. The effect of CNT radius on the thermal conductivity of the composite has been found to be almost similar for both values of CNT length, i.e. $L_c = 40$ and 50 nm. From the results shown in Figure 4, it can be concluded that the results obtained by EFG method are almost similar with those obtained by proposed formula, whereas the results obtained by existing formula are unreliable for this study. Since, in existing formula, the effect of nanotube radius has not been considered properly.

4.4 Effect of RVE length (L) on thermal conductivity

In this sub-section, the effect of RVE length on the equivalent thermal conductivity of the composites has been studied in detail. Various modeling parameters required to study the effect of RVE length on the equivalent thermal conductivity of the composite, are tabulated in Table I. Different values of RVE length, i.e. from 80 to 130 nm have been taken to study the effect of RVE length. Figure 5 shows the variation in equivalent thermal conductivity of the composite with RVE length. For $L = 80$ and 130 nm with $L_c = 50$ nm, the volume fractions are 11.5 and 7.0 per cent, and their

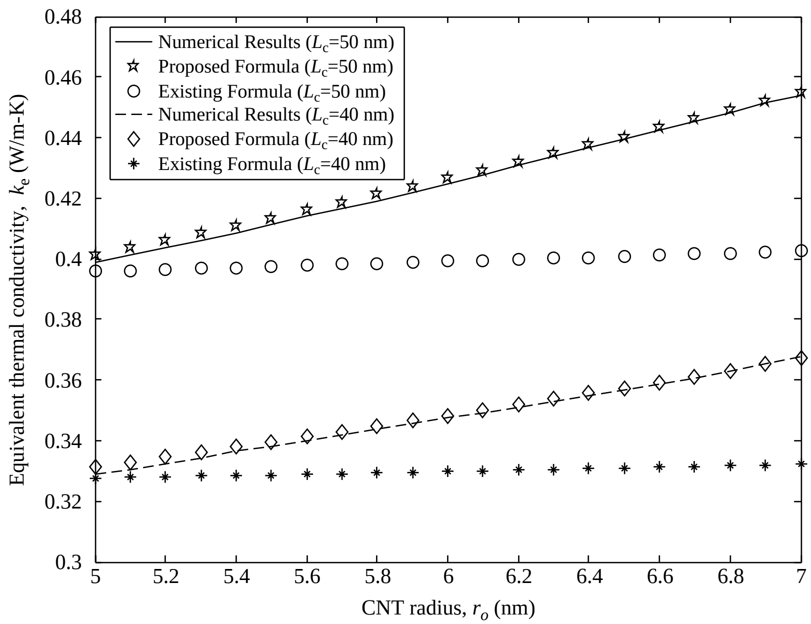

Figure 4.
Variation of equivalent thermal conductivity with CNT radius

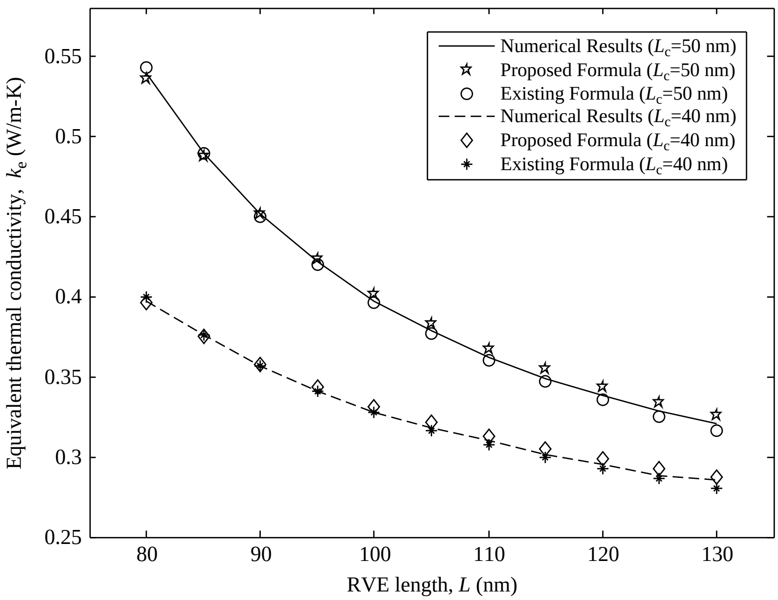

Figure 5.
Variation of equivalent thermal conductivity with RVE length

corresponding equivalent thermal conductivities are 2.84 and 1.69 times that of polymer matrix, respectively, whereas for same values of L with $L_c = 40$ nm, the volume fractions are 13.9 and 8.6 per cent, and their corresponding equivalent thermal conductivities are 2.10 and 1.50 times that of polymer matrix, respectively. The results obtained by numerical method and proposed formula have also been compared with those obtained by existing formula.

4.5 Effect of RVE radius (R_o) on thermal conductivity

Various modeling parameters required to study the effect of RVE radius on the equivalent thermal conductivity of the composite are tabulated in Table I. The equivalent thermal conductivity of the composite has been evaluated by EFG method, proposed formula and existing formula for various values of RVE radius. The effect of RVE radius has been studied for two values of CNT lengths, i.e. $L_c = 40$ and 50 nm, and are shown in Figure 6. Adding 14.2 per cent (equivalent to $R_c = 10$ nm and $L_c = 50$ nm) of CNT increases the equivalent thermal conductivity of the composite to 0.4176 W/m-K, whereas 3.5 per cent (equivalent to $R_c = 20$ nm and $L_c = 50$ nm) of CNT addition increases the equivalent thermal conductivity of the composite to 0.3176 W/m-K. From the results shown in Figure 6, it can be noted that the equivalent thermal conductivity of the composite decreases with the increase in RVE radius for both values of CNT length. In existing approximate formula, thermal conductivity has not been considered a function of RVE cross-sectional dimension, i.e. radius in present study; thereby, the results obtained by existing formula are totally unreliable for this study.

5. Conclusions

In this paper, meshless EFG method was successfully applied to evaluate the thermal properties of CNT-composites. The results were obtained using cylindrical representative

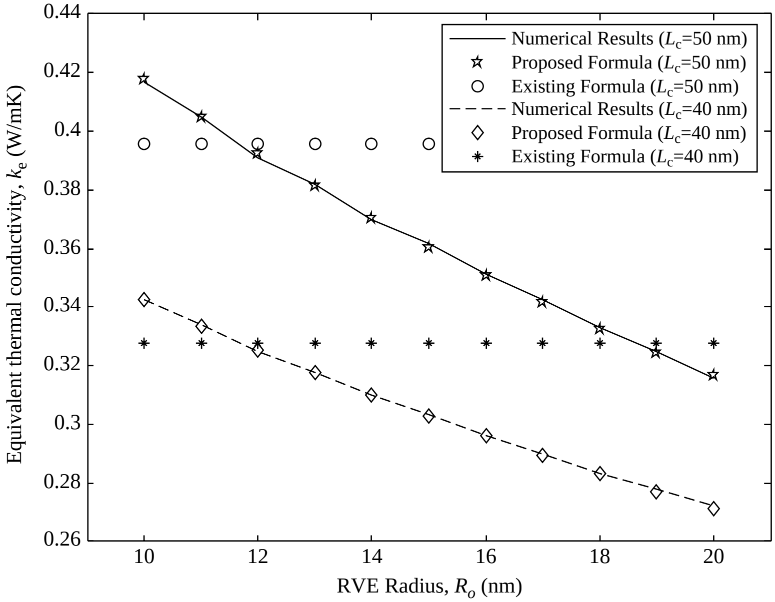

Figure 6.
Variation of equivalent thermal conductivity with RVE radius

volume element for a model problem. The equivalent thermal conductivity of the composite was evaluated using continuum mechanics approach, and plotted against various model parameters. Present computations show that the thermal conductivity of CNT-composites is a function of CNT length, CNT radius, RVE length and RVE radius. The addition of 16.1 per cent of CNT increases the equivalent thermal conductivity of the composite by 352 per cent. An approximate formula was also proposed to evaluate the equivalent thermal conductivity of carbon nanotube composites. The results obtained by proposed approximate formula were found in good agreement with those obtained by numerical simulation.

References

Belytschko, T., Lu, Y.Y. and Gu, L. (1994), "Element free Galerkin methods", *International Journal for Numerical Methods in Engineering*, Vol. 37, pp. 229-56.

Bower, C., Rosen, R., Jin, L., Han, J. and Zhou, O. (1999), "Deformation of carbon nanotubes in nanotube – polymer composites", *Applied Physics Letters*, Vol. 74, pp. 3317-9.

Chen, X.L. and Liu, Y.J. (2004), "Square representative volume elements for evaluating the effective material properties of carbon nanotube-based composites", *Computational Materials Science*, Vol. 29, pp. 1-11.

Liu, Y.J. and Chen, X.L. (2003a), "Continuum models of carbon nanotube-based composites by the BEM", *Electronic Journal of Boundary Elements*, Vol. 1, pp. 316-35.

Liu, Y.J. and Chen, X.L. (2003b), "Evaluations of the effective materials properties of carbon nanotube-based composites using a nanoscale representative volume element", *Mechanics of Materials*, Vol. 35, pp. 69-81.

Liu, Y.J., Nishimura, N. and Otani, Y. (2005a), "Large-scale modeling of carbon-nanotube composites by fast multipole boundary element method", *Computational Materials Science*, Vol. 34, pp. 173-87.

Liu, Y.J., Nishimura, N., Otani, Y., Takahasi, T., Chen, X.L. and Munakata, H. (2005b), "A fast boundary element method for the analysis of fiber-reinforced composites based on a rigid inclusion model", *ASME Journal of Applied Mechanics*, Vol. 72, pp. 115-28.

Nishimura, N. and Liu, Y.J. (2004), "Thermal analysis of carbon-nanotube composites using a rigid-line inclusion model by the boundary integral equation method", *Computational Mechanics*, Vol. 35, pp. 1-10.

Qian, D., Dickey, E.C., Andrews, R. and Rantell, T. (2000), "Load transfer and deformation mechanisms in carbon nanotube–polystyrene composites", *Applied Physics Letters*, Vol. 76, pp. 2868-70.

Schadler, L.S., Giannaris, S.C. and Ajayan, P.M. (1998), "Load transfer in carbon nanotube epoxy composites", *Applied Physics Letters*, Vol. 73, pp. 3842-4.

Singh, I.V., Sandeep, K. and Prakash, R. (2004), "Application of meshless element free Galerkin method in two-dimensional heat conduction problems", *Computer Assisted Mechanics and Engineering Sciences*, Vol. 11, pp. 265-74.

Song, Y.S. and Youn, J.R. (2006), "Evaluation of effective thermal conductivity for carbon nanotube/polymer composites using control volume finite element method", *Carbon*, Vol. 44, pp. 710-7.

Srivastava, D., Menon, M. and Cho, K. (2001), "Computational nanotechnology with carbon nanotubes and fullerenes", *Computing in Science and Engineering*, Vol. 3, pp. 42-55.

Tanaka, Masa., Zhang, J. and Matsumoto, T. (2003), "Multi-domain hybrid BNM for predicting thermal properties of CNT composites", paper presented at Asia-Pacific International Conference on Computational Methods in Engineering, Sapporo, 5-7 November, pp. 3-12.

Wagner, H.D., Lourie, O., Feldman, Y. and Tenne, R. (1998), "Stress induced fragmentation of multi wall carbon nanotubes in a polymer matrix", *Applied Physics Letters*, Vol. 72, pp. 188-90.

Zhang, J., Tanaka, M. and Matsumoto, T. (2004a), "A simplified approach for heat conduction analysis of CNT-based nano composites", *Computer Methods in Applied Mechanics and Engineering*, Vol. 193, pp. 5597-609.

Zhang, J., Tanaka, M., Matsumoto, T. and Guzik, A. (2004b), "Heat conduction analysis in bodies containing thin walled structures by means of hybrid BNM with an application to CNT-based composites", *JSME International Journal*, Vol. 47, pp. 181-8.

Further reading

Singh, I.V. (2004), "Meshless EFG method in 3-D heat transfer problems: a numerical comparison, cost and error analysis", *Numerical Heat Transfer-Part A*, Vol. 46, pp. 192-220.

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