HEAT CONDUCTION ANALYSIS OF CNT BASED NANO-COMPOSITES BY FINITE ELEMENT AND ELEMENT FREE GALERKIN METHODS

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This paper deals with the heat conduction analysis of CNT based nano-composites by finite element and element free Galerkin methods. The thermal properties of these composites have been evaluated by continuum mechanics approach using cylindrical representative volume element. The values of temperature and heat flux have been calculated at few typical locations and plotted against RVE length. The present computations show that by addition of 3.5% (by volume) of CNT in polymer matrix, results in an increase of thermal conductivity by 30.8% for EFG method & 28.4% for finite element method whereas by addition of 8.5% (by volume) of CNT, results in an increase of thermal conductivity by 206.7% & 203.2% for EFG and finite element methods respectively. The results obtained by EFG method have been compared with those obtained by finite element method and have been found in good agreement with each other.

Keywords: Carbon nanotube; nano-composites; thermal conductivity; finite element method and EFG method

1. Introduction

Over past 10 years, carbon nanotubes (CNTs) have gained the interest of many scientists and researchers towards the field of nanotechnology due to their excellent mechanical, electrical and thermal properties. These remarkable properties of CNTs are responsible for the intensive research which has been carried out in last decade. Endo and his co-workers [1] have analyzed the physical properties, production methodology and possible applications of CNTs. Many researchers have studied their mechanical properties by experimental work [2-5] and by numerical simulations [6-11]. Since, an experiment provides us various properties as well as reasons to posses these properties whereas numerical simulations help us in analyzing and designing of nano-composites. It has been found that by addition of only 1% (by weight) of CNTs in a matrix, the stiffness of the resulting composite increases by 36-42% and tensile strength by 25% [11].

The prediction of thermal behavior of nano-materials is the current need of today's world due to continuous reduction of device size. In this regard, few experiments were conducted on compressed ropes of CNTs [12-13] and the thermal conductivity was found to be in the range of 1750 to 5850 W/m K. By direct experiment, the thermal conductivity of an individual multi-walled CNT was found to be 3000 W/m K [15] at room temperature. An even higher value of thermal conductivity was reported by numerical simulations based on molecular dynamics (MD) approach [16-18] i.e. 6600 W/m K at room temperature (300 K). Biercuk et al. [18] found that by addition of only 1% (by weight) single walled nanotubes results an increase of heat conductivity by 70% at 40 K and by 125% at room temperature. Almost all these studies on thermal conductivities were based on molecular dynamics (MD) approach but these approaches are limited to very small length & time scales and can not deal with large scale problems due to limitation of current computing facility. Recently some studies were also carried out based on continuum mechanics approach. Zhang et al. [19-21] used the meshless hybrid boundary node method (hybrid BNM) for the heat conduction analysis of CNT based nano-composites. They used multi-domain & simplified approaches to predict the thermal properties of nano-composites and also coupled their method with fast multipole method to solve large scale problems. In their study, it was found that by addition of 7.2% (by volume) of CNTs in the polymer matrix results in 49% increase of thermal conductivity of the composite. In the continuity of continuum mechanics approach, Nishimura and Liu [22] applied the boundary integral equation (BIE) method for the thermal analysis of CNT based nano-composites. They analyzed a heat conduction problems in two-dimensional infinite domain embedded with many rigid inclusions with the help of a fast multipole boundary element method.

Till date only boundary type methods such as BEM and hybrid BNM were used to predict the thermal behavior of CNT based composites. In these boundary type methods, square representative volume element (square RVE) was used to obtain the thermal properties but these methods do not posses symmetry and bandedness properties in their solution matrix; therefore, the solution of large scale problems becomes a time consuming and burdensome task as compared with domain type methods such as finite element method (FEM) and element free Galerkin (EFG) method. Although, fast multipole method (FMM) can alleviate the difficulty to solve large scale problems by some extend but its implementation is also an intricate task. Therefore, the search for an ideal method remains still continued to predict the thermal behavior of nano-composites. As such both FEM and EFG method posses symmetry and bandedness properties in their solution matrix and can be easily extended to solve large scale problems. Therefore, in the present work an attempt has been made to extend the domain type EFG and finite element methods to solve CNT based nano-composite problems. A nanoscale cylindrical representative volume element (cylindrical RVE) has been used to evaluate the thermal properties of composites by continuum mechanics approach. The temperature and heat flux distributions have been plotted as function of RVE length at few typical locations. The thermal conductivity has been evaluated and plotted for various CNT lengths. The results obtained by EFG and finite element methods have been compared with each other and have been found in good agreement.

2. Review of EFG Method

The meshless element free Galerkin (EFG) method requires moving least square (MLS) approximations for the discretization of the governing equations. These MLS approximations consist of three components: a weight function associated with each node, a basis function and a set of constant coefficients that depends on node position. Using MLS approximation scheme, an unknown function of temperature $T(\mathbf{r})$ is approximated as $T^h(\mathbf{r})$ [23].

$$T^h(\mathbf{r}) = \sum_{I=1}^{n} \Phi_I(\mathbf{r}) T_I = \mathbf{\Phi}(\mathbf{r})\mathbf{T} \tag{1}$$

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

$$\Phi_I(\mathbf{r}) = \sum_{j=1}^{m} p_j(\mathbf{r})(\mathbf{A}^{-1}(\mathbf{r})\mathbf{B}(\mathbf{r}))_{jI} = \mathbf{p}^T\mathbf{A}^{-1}\mathbf{B}_I \tag{2a}$$

where,

$$\mathbf{A}(\mathbf{r}) = w(\mathbf{r}-\mathbf{r}_1)\begin{bmatrix} 1 & r_1 & z_1 \\ r_1 & r_1^2 & r_1 z_1 \\ z_1 & r_1 z_1 & z_1 \end{bmatrix} + \ldots w(\mathbf{r}-\mathbf{r}_n)\begin{bmatrix} 1 & r_n & z_n \\ r_n & r_n^2 & r_n z_n \\ z_n & r_n z_n & z_n \end{bmatrix} \tag{2b}$$

$$\mathbf{B}(\mathbf{r}) = \left\{ w(\mathbf{r}-\mathbf{r}_1)\begin{bmatrix} 1 \\ r_1 \\ z_1 \end{bmatrix}, \ldots\ldots\ldots w(\mathbf{r}-\mathbf{r}_n)\begin{bmatrix} 1 \\ r_n \\ z_n \end{bmatrix} \right\} \tag{2c}$$

The rational weight function [24] has been used in this work, which is given as

$$w(s) = \begin{cases} \dfrac{1}{s^{\bar{n}} + C} & 0 \le s \le 1 \\ 0 & s > 1 \end{cases} \tag{3}$$

where, $2 \le \bar{n} \le 7$, $0.01 \le C \le 0.1$, $s = \dfrac{\| \mathbf{r} - \mathbf{r}_I \|}{d_{mI}}$ is the normalized radius, $d_{mI} = d_{\max} c_I$ and $d_{\max}$ = scaling parameter (for complete details of EFG method, refer to article by Belytschko et al. [25]).

3. Numerical Implementation of EFG Method

Carbon nanotubes (CNTs) behave as a superconductor in nano-composites due to their very high value of thermal conductivity as compared to polymer matrix. Zhang et al. [19] evaluated the thermal properties of these composites using hybrid BNM and they predicted an almost constant temperature distribution on CNT surface. In the present work, heat conduction analysis of nano-composites has been carried out using cylindrical RVE by assuming CNT at a constant temperature. A model containing single CNT inside the cylindrical RVE has been taken for the thermal analysis. Both ends of RVE are subjected to constant temperatures & outer surface is kept insulated. Hence, this problem can be treated as an axisymmetric heat transfer problem governed by the steady sate heat conduction equation in cylindrical coordinate system

$$k_r \frac{\partial T}{\partial r^2} + \frac{k_r}{r}\frac{\partial T}{\partial r} + k_z \frac{\partial T}{\partial z} = 0 \tag{4a}$$

with the following essential boundary conditions

$$\text{at } z = 0, \qquad T = T_{\mathrm{L}} \tag{4b}$$

$$\text{at } z = L, \qquad T = T_{\mathrm{R}} \tag{4c}$$

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

$$\int_{\Omega} \bar{w}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(k_r\, r\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right)\right] 2\pi\, r\, dr\, dz = 0 \tag{5}$$

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

$$2\pi \int_{\Omega} (k\,\bar{w}_{,r} T_{,r} + k\,\bar{w}_{,z} T_{,z})\, r\, dr\, dz - 2\pi \int_{\Gamma} \bar{w}\, r\, q\, d\Gamma = 0 \tag{6}$$

where, $q = k\,T_{,r}\cos(n',r) + kT_{,z}\cos(n',z)$ and $k_r = k_z = k$

From Eq. (6), the functional $I(T)$ can be obtained as

$$I(T) = \pi \int_{\Omega} k(T_{,r}^{\;2} + T_{,z}^{\;2})\; r\, dr\, dz \tag{7}$$

Enforcing essential boundary conditions using Lagrange multiplier method, the functional $I^*(T)$ is obtained as

$$\begin{aligned} I^*(T) = \pi &\int_{\Omega} k(T_{,r}^{\;2} + T_{,z}^{\;2})\, r\, dr\, dz + \\ &\int_{\Gamma_L} \lambda_L (T - T_L)\, d\Gamma + \int_{\Gamma_R} \lambda_R\, (T - T_R)\, d\Gamma \end{aligned} \tag{8}$$

Taking variation i.e. $\delta I^*(T)$ of Eq. (8), it reduces to

$$\begin{aligned} \delta I^*(T) = 2\pi &\int_{\Omega} k(T_{,r}^{\;T}\delta T_{,r} + T_{,z}^{\;T}\delta T_{,z})\, r\, dr dz \\ &+ \int_{\Gamma_L} \lambda_L\; \delta T\, d\Gamma + \int_{\Gamma_L} \delta\lambda_L\, (T - T_L)\, d\Gamma \\ &+ \int_{\Gamma_R} \lambda_R\; \delta T\, d\Gamma + \int_{\Gamma_R} \delta\lambda_R\, (T - T_R)\, d\Gamma \end{aligned} \tag{9}$$

Since $\delta I^*(T) = 0$ and δT, $\delta\lambda_L$ & $\delta\lambda_R$ are arbitrary in Eq. (9), hence it can be written in the following form using Eq. (1)

$$\begin{bmatrix} \mathbf{K} & \mathbf{G}_L & \mathbf{G}_R \\ \mathbf{G}_L^{\;T} & 0 & 0 \\ \mathbf{G}_R^{\;T} & 0 & 0 \end{bmatrix} \begin{Bmatrix} \mathbf{T} \\ \boldsymbol{\lambda}_L \\ \boldsymbol{\lambda}_R \end{Bmatrix} = \begin{Bmatrix} \mathbf{f} \\ \mathbf{f}_L \\ \mathbf{f}_R \end{Bmatrix} \tag{10a}$$

where,

$$K_{IJ} = 2\pi \int_{\Omega} \begin{bmatrix} \Phi_{I,r} \\ \Phi_{I,z} \end{bmatrix}^T \begin{bmatrix} k & 0 \\ 0 & k \end{bmatrix} \begin{bmatrix} \Phi_{I,r} \\ \Phi_{I,z} \end{bmatrix} r\, dr dz \tag{10b}$$

$$f_I = 0 \tag{10c}$$

$$(G_L)_{IK} = \int_{\Gamma_L} \Phi_I N_K \, d\Gamma \tag{10d}$$

$$(f_L)_K = \int_{\Gamma_L} T_L N_K \, d\Gamma \tag{10e}$$

$$(G_R)_{IK} = \int_{\Gamma_R} \Phi_I N_K \, d\Gamma \tag{10f}$$

$$(f_R)_K = \int_{\Gamma_R} T_R N_K \, d\Gamma \tag{10g}$$

Introducing another essential boundary condition at the CNT surface using Lagrange multiplier method, the Eq. (10a) is modified as

$$\begin{bmatrix} \mathbf{K} & \mathbf{G}_L & \mathbf{G}_R & \mathbf{G}_c \\ \mathbf{G}_L^T & 0 & 0 & 0 \\ \mathbf{G}_R^T & 0 & 0 & 0 \\ \mathbf{G}_c^T & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \mathbf{T} \\ \boldsymbol{\lambda}_L \\ \boldsymbol{\lambda}_R \\ \boldsymbol{\lambda}_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f} \\ \mathbf{f}_L \\ \mathbf{f}_R \\ \mathbf{f}_c \end{Bmatrix} \tag{11a}$$

where,

$$(G_c)_{IK} = \int_{\Gamma_c} \Phi_I N_K \, d\Gamma \tag{11b}$$

$$(f_c)_K = \int_{\Gamma_c} T_c N_K \, d\Gamma \tag{11c}$$

Since T_c is unknown in Eq. (11c), hence Eq. (11a) is further written as

$$\begin{bmatrix} \mathbf{K} & \mathbf{G}_L & \mathbf{G}_R & \mathbf{G}_c & 0 \\ \mathbf{G}_L^T & 0 & 0 & 0 & 0 \\ \mathbf{G}_R^T & 0 & 0 & 0 & 0 \\ \mathbf{G}_c^T & 0 & 0 & 0 & -\mathbf{f}_c' \end{bmatrix} \begin{Bmatrix} \mathbf{T} \\ \boldsymbol{\lambda}_L \\ \boldsymbol{\lambda}_R \\ \boldsymbol{\lambda}_c \\ T_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f} \\ \mathbf{f}_L \\ \mathbf{f}_R \\ 0 \end{Bmatrix} \tag{12a}$$

$$\text{where, } (f_c')_K = \int_{\Gamma_c} N_K \, d\Gamma \tag{12b}$$

Now in Eq. (12a), there is one additional unknown T_c which requires one more equation to solve the system of equations. This additional equation has been obtained by using law of conservation of energy at the CNT surface i.e. (net rate of thermal energy flowing through CNT surface is zero), which is given by

$$\int_{\Gamma_c} q \, d\Gamma = 0 \tag{13}$$

where, $q = k\, T_{,r} \cos(n', r) + k T_{,z} \cos(n', z)$

Introducing $\int_{\Gamma_c} q \, d\Gamma = 0$ in Eq. (12a)

$$\left[\begin{array}{cccc|c} \mathbf{K} & \mathbf{G}_L & \mathbf{G}_R & \mathbf{G}_c & 0 \\ \mathbf{G}_L^T & 0 & 0 & 0 & 0 \\ \mathbf{G}_R^T & 0 & 0 & 0 & 0 \\ \mathbf{G}_c^T & 0 & 0 & 0 & -\mathbf{f}_c' \\ \hline \mathbf{f}_c'' & 0 & 0 & 0 & 0 \end{array}\right] \begin{Bmatrix} \mathbf{T} \\ \boldsymbol{\lambda}_L \\ \boldsymbol{\lambda}_R \\ \boldsymbol{\lambda}_c \\ T_c \end{Bmatrix} = \begin{Bmatrix} \mathbf{f} \\ \mathbf{f}_L \\ \mathbf{f}_R \\ 0 \\ 0 \end{Bmatrix} \tag{14}$$

where, $(f_c'')_I = \int_{\Gamma_c} \left[k\Phi_{,r} \cos(n', r) + k\Phi_{,z} \cos(n', z) \right] d\Gamma$ with n' is the outward normal to the CNT surface

4. Results and Discussion

In this section, a model problem has been solved by finite element and element free Galerkin methods. A nanoscale cylindrical representative volume element containing single nanotube (as shown in Fig. 1) has been taken as a model problem to study the thermal behavior of nano-composites. CNT is placed symmetrically at the center of RVE such that the axis of RVE and CNT are coinciding each other.

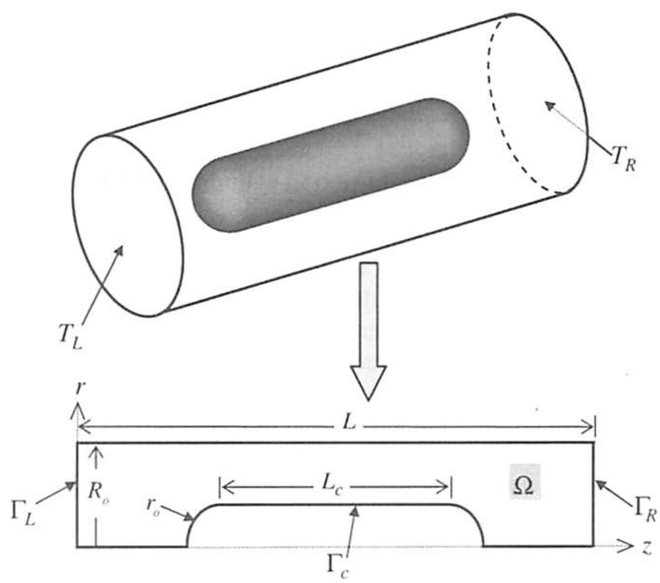

Fig. 1: Nano scale representation of a CNT problem

Table 1: Data for CNT based composite problem

Parameter	Value of parameter
RVE length, L	100 nm
Nanotube length, L_c	50 nm
RVE radius, R_o	15 nm
Nanotube outer radius, r_o	5 nm
Nanotube thickness, t	0.4 nm
Thermal conductivity of matrix , k	0.37 W/m K
Temperature at Γ_L, T_L	200 K
Temperature at Γ_R, T_R	100 K

The ends of RVE are maintained at two different temperatures and outer cylindrical surface is made flux free. The data used for the heat conduction analysis of the composite model is tabulated in Table 1. The EFG results have been obtained by treating the model problem as an axisymmetric heat transfer problem governed by Laplace equation. Lagrange multiplier approach has been used to enforce the essential boundary conditions. The FEM results have been obtained by commercial ANSYS Package (Version 9.0). Ten noded tetrahedral elements (solid 87) have been used to obtain the FEM solution. Assuming material properties as homogeneous, isotropic and independent of temperature, the equivalent thermal conductivity of the composite is evaluated as

$$k_e = -\frac{qL}{\Delta T} \tag{15}$$

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.
The volume fraction of CNT has been calculated by the following expression

$$v = \left(\frac{V_c}{V_c + V_m} \right) \tag{16}$$

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

4.1 Temperature Distribution in cylindrical RVE

The temperature distribution inside RVE has been studied at two typical locations of RVE radius i.e. r = 5.25 & 14.75 nm. The temperature values obtained by EFG & finite element methods are presented in Fig. 2 at the location r =5.25 nm. From the results presented in Fig. 2, it has been noticed that the temperature first decreases rapidly from left end of RVE (200K) to the left end of CNT (150 K) after that it almost remains constant (150 K) along CNT length then it again start decreasing from right end of CNT (150 K) to the other end of RVE (100 K).

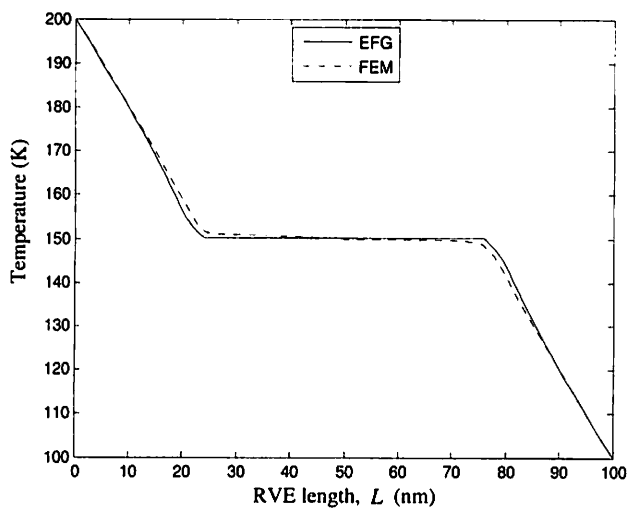

Fig. 2: Temperature variation with RVE length (L) at r =5.25 nm

The variation of temperature with RVE length is also presented in Fig. 3 at another location r =14.75 nm and almost similar behavior has been observed. Based on the results presented in Fig. 2 and Fig. 3, it can be stated that the most of the heat flux passes through the nanotube only. Moreover, the temperature values obtained by EFG and FE approaches have been found in good conformity with each other.

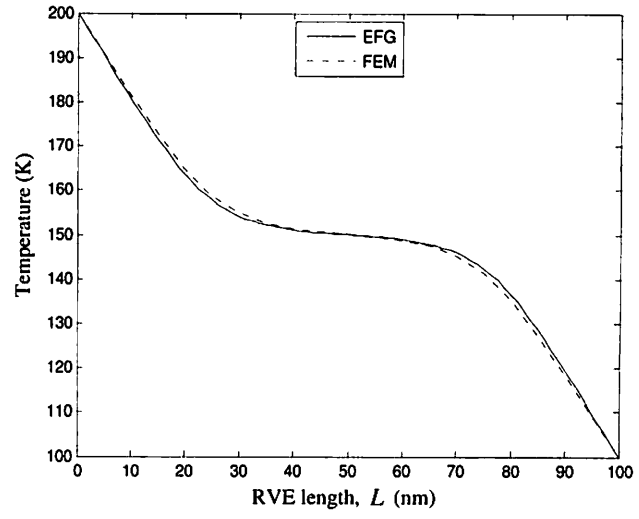

Fig. 3: Temperature variation with RVE length (L) at r =14.75 nm

4.2 Heat Flux Distribution in cylindrical RVE

The data required for the study of heat flux inside RVE is presented in Table 1. The heat flux values have been obtained by EFG and FE approaches at two typical locations of RVE radius. Fig. 4 shows a variation of heat flux with RVE length at the location r =5.25 nm. From the results presented in Fig. 4, it has been observed that the variation in heat flux is small for the some portion of RVE after that it rapidly drops to almost zero value then it nearly remains constant (nearly zero) for the CNT length of RVE and finally approaches to its initial value.

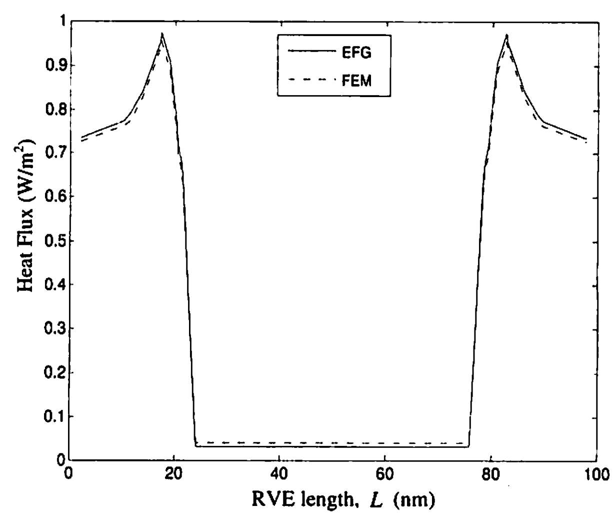

Fig. 4: Variation of heat flux with RVE length (L) at r =5.25 nm

An almost similar behavior of heat flux with RVE length has been observed in Fig. 5 at the location r =14.75 nm. From the results presented in Fig. 4 and Fig, 5, it has been clearly observed that almost entire heat flux passes through the nanotube. The results obtained by EFG method have been found in good agreement with those obtained by finite element method.

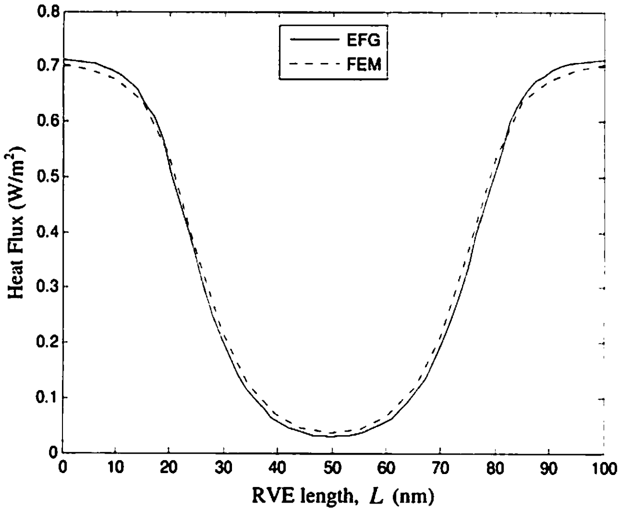

Fig. 5: Variation of heat flux with RVE length (L) at r =14.75 nm

4.3 Variation of Equivalent Thermal Conductivity (k_e) with CNT length (L_c)

This sub-section describes the effect of CNT length on the equivalent thermal conductivity (k_e) of the composites. The parameters required for this study are given in Table 1, except the value of CNT length. The values of thermal conductivity have been evaluated by EFG and finite element methods. Various values of CNT length (from 25 nm to 70 nm) have been selected to study the effect of CNT length on thermal conductivity. Fig. 6 shows the variation of equivalent thermal conductivity with CNT length. For L_c = 25 nm (3.5% by volume), the increase in the values of thermal conductivities obtained by EFG and finite element approaches has been found to be 30.8% and 28.4% respectively whereas for L_c = 70 nm (8.5% by volume), the increase in values of thermal conductivities are observed to be 206.7% and 203.3% respectively. The above analysis shows that the results obtained by EFG and finite element methods have been found in good concurrence with each other.

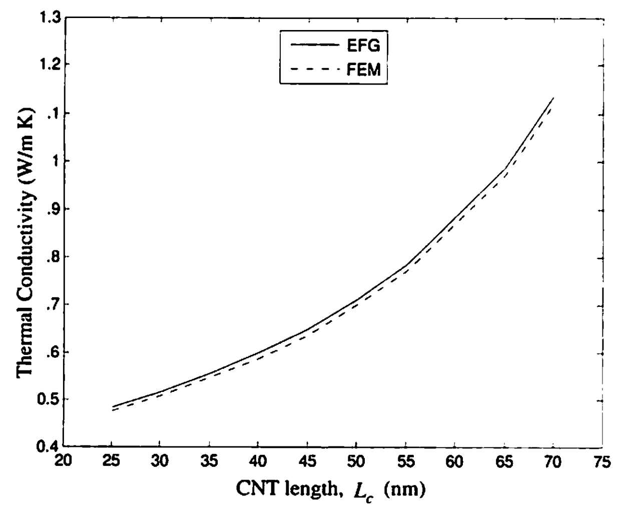

Fig. 6: Variation of equivalent thermal conductivity (k_e) with nanotube length (L_c)

5. Conclusions

In this work, domain type meshless EFG and finite element methods have been used for the heat conduction analysis of nano-composites. The numerical simulation has been carried out using continuum mechanics approach. Present simulation shows that by addition of 3.5% (by volume) of CNT results in nearly 30% increase in the thermal conductivity of the polymer matrix whereas by addition of 8.5% (by volume) of CNT increases the thermal conductivity of the matrix approximately by 205%. The results obtained by EFG method have been compared with those obtained by FEM and have been found in good agreement with each other. Due to symmetry & bandedness properties in the solution matrix, the meshless EFG method can be easily extended to predict the thermal properties of CNT based nano-composites with large number of arbitrary shaped CNTs randomly distributed in the polymer matrix.

Notations

k thermal conductivity of matrix, W/m K
k_e equivalent thermal conductivity of composite, W/m K
L length of cylindrical RVE, nm
L_c CNT length, nm
m number of terms in basis
n number of nodes in the domain of influence
n' outward normal to the surface
N_K Lagrange Interpolant
q heat flux, W/m^2
r_o outer radius of CNT, nm
R_o radius of cylindrical RVE, nm
t thickness of CNT, nm
T_c constant temperature at CNT surface, K
$T^h(\mathbf{r})$ MLS approximation function for temperature
w weight function used in MLS approximation
$\overline{w}$ weighting function used in weighted integral form
Γ_c CNT boundary surface
Γ boundary of the domain
Ω computational domain
$\Phi_I(\mathbf{r})$ shape function

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