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Numerical Analysis of Heat Transfer of Polyethylene Nanocomposites with Carbon Nanotubes

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ABSTRACT

Nanotechnology, with its gigantic nature, has broken the boundaries of different branches of science and provided the basis for using the results and possibilities in many areas to improve the quality of life. This approach will help you systematically investigate the impact of volume percentage and aspect ratio on the thermal conductivity coefficient of carbon nanotube nanoparticles within a Representative Volume Elements (RVE) using Monte Carlo simulations in MATLAB. The aim of this study was to model the thermal conductivity of polyethylene-based composite reinforced with helical carbon nanotubes using the finite element method. It shows that the heat conduction coefficient value increases with the increase in the volume percentage, aspect ratio, and radius of helical nanoparticles, and this increase is the most effective factor for the volume percentage between 0.73% and 9.5%.

Keywords: Finite elements, helical carbon nanotubes, nano, nanocomposite

INTRODUCTION

The findings regarding the thermal behavior of nanocomposite materials with carbon nanotubes (CCNTs) have broader implications that significantly contribute to the field of nanocomposite materials and various related areas. Here are some of the broader implications:

Advanced Material Design

The research findings enable the development of advanced nanocomposite materials with tailored thermal properties. This contributes to the field by expanding the toolkit for material scientists and engineers, allowing them to design materials with enhanced thermal performance for specific applications.

Improved Thermal Management

Nanocomposite materials with optimized thermal behavior can be used to address thermal management challenges in a wide range of industries, including electronics, aerospace, automotive, and energy storage. This has the potential to improve the efficiency, reliability, and life span of various devices and systems.

Energy Efficiency and Sustainability

The ability to create nanocomposites with improved thermal properties can lead to more energy-efficient technologies, reducing energy consumption and greenhouse gas emissions. This aligns with global sustainability goals and contributes to the development of environmentally friendly solutions.

Materials for Emerging Technologies

Emerging technologies, such as 5G, electric vehicles, and renewable energy systems, often require advanced thermal management solutions. The findings offer insights into developing materials that can meet the demanding requirements of these technologies.

Phonon Engineering

Understanding how parameters like defects and functionalization impact phonon behavior in nanocomposites provides a foundation for phonon engineering. This is critical for the development of materials that can control and manipulate heat conduction, not only in nanocomposites but also in other materials and devices.

Multidisciplinary Collaboration

Research in the field of nanocomposite materials involves collaboration between materials scientists, physicists, chemists, and engineers. The findings encourage multidisciplinary efforts to address complex challenges and develop innovative solutions.

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Nanotechnology Advancements
The research contributes to the broader field of nanotechnology by expanding our understanding of how nanoscale materials like CCNTs can be harnessed to improve the properties of macroscopic materials. This knowledge can be applied to other nanomaterials and nanostructures.

Economic and Industrial Impact
Industries and companies involved in the production and application of nanocomposite materials can benefit from the development of more efficient and effective products. This can lead to economic growth and competitiveness in various markets.

In summary, the findings regarding the thermal behavior of nanocomposite materials with CCNTs have far-reaching implications, not only in the field of materials science but also in addressing real-world challenges related to energy efficiency, sustainability, and the advancement of emerging technologies. This research contributes to the development of innovative solutions and has the potential to positively impact multiple industries and sectors.

Nano comes from the Greek root "nance," meaning dwarf.[1] Nanotechnology, the fourth wave of the industrial revolution, is a huge phenomenon that has entered all scientific trends to the extent that the superiority of processes will be revealed in the next decade and will depend on this development.[2] The nature of nanotechnology is the ability to work at atomic, molecular, and beyond levels, using the arrangement of atoms or molecules to arrange and manipulate atoms or molecules in sizes between 1 and 100 nanometers. Replacing these structures with materials, devices, and systems with new capabilities and ensuring the higher efficiency of materials. Nanotechnology is the process of producing materials and tools by manipulating materials at the atomic scale and controlling them at the atomic and molecular level. In fact, if all materials and systems organize their basic structures at the nanoscale, then all reactions will be carried out faster and more optimally, and sustainable development will be realized.[1] Among the many achievements of this technology, the use of energy with high efficiency in its production, transmission, consumption, and storage will also be created, leading to a tremendous transformation in this field.[2] Practitioners and researchers of nanoscience are therefore trying to use this technology to provide greater comfort and well-being inside and outside the building by finding a new class of high-performance building materials, saving money on costs, especially the consumption of energy resources, and finally ensuring sustainable development. Nanotechnology will lead to dramatic changes in the use of natural resources, energy and water, and reducing waste and pollution.

Adding nanoparticles such as graphene nanosheets, CCNTs, helical CCNTs, clay nanoparticles, and metal oxide nanoparticles to the matrix generally increases the electrical, mechanical, material, magnetic, and optical properties. Due to its special geometric shape, significant surface-to-volume ratio, and high mechanical and thermal properties, the use of CCNT nanoparticles will increase the nanocomposite's resistance to destruction and fracture, as well as its thermal and mechanical properties.[3-6] Among carbon nanotubes, helical carbon nanotubes, which have the mechanical, thermal, and electrical properties of carbon nanotubes, have recently become the focus of researchers' attention due to their geometric structure. Carbon nanotubes were predicted by Dunlap in 1990.[7,8] Carbon nanotubes and helical carbon nanotubes are anisotropic materials, but they are assumed to be isotropic in many studies[9,10] and in this study as well. Based on this brief description of CCNTs, the following provides an overview of previous research. Using the finite element method, the elastic properties of CCNT polymeric nanocomposite, as well as the effect of CCNT geometric parameters, number, aspect ratio, volume fraction, and interphase, were investigated and obtained by Koc et al.[11]

Mehrdad Shokrieh et al[12] showed that mechanical loading improved the effective thermal resonance coefficient and increased the elastic modulus of the nanocomposite. Mehrdad Shokrieh et al.[12] numerically examined how the length of the RVE affected the mechanical properties of the nanocomposite they produced. Their findings showed that, at a fixed volume percentage, the length or width of the RVE has a big impact on the nanocomposite's longitudinal elastic modulus.

In an analytical study, Tran[13] has a simple approach to obtain the effective heat conduction coefficient. They presented a two- and three-dimensional multiphase composite that envisions even high-volume percentages of nanoparticles. Finally, the theoretical results of his model had good agreement with the laboratory and finite element results of others.

Lu[14] conducted one of the first studies examining the elastic properties of single-walled and multiwalled CNTs using binary harmonic potentials. In this study, the interaction between tubes in MNCNTs was taken into account with van der Waals forces.

Yetgin et al[15] examined the tribological and mechanical properties of graphite-added polypropylene composites in their study. For their studies, they added 1%, 3%, 5%, and 10% graphite by weight to the polypropylene polymer.

Sever et al[16] stated in their study that a large amount of agricultural waste is generated in the world as a result of agricultural harvests and pruning. They mentioned that very few of these wastes were converted and used as agricultural fertilizer and fuel, and the remaining were not utilized. In this regard, many studies have recently been carried out to combine fullerenes and CNTs.[17-23]

According to a review of previous studies, so far no study has been reported in the sources that investigates the effect of CCNT nanoparticles on the effective thermal conductivity coefficient of nanocomposites. Ethylene's effective thermal conductivity coefficient is obtained by the two-dimensional finite element method. In this study, the assumption of a complete connection between the nanoparticles and the polymer was taken into account, and the electrical resistance between the nanoparticles and the matrix was also ignored. First of all, using a program written in MATLAB software, CCNT nanoparticles spread isotropically in the RVE with the Monte Carlo algorithm. After obtaining the appropriate RVE length, a parametric study is carried out; the effect of volume percentage and aspect ratio on the thermal conductivity coefficient of CCNT nanoparticles is investigated.

MATERIAL AND METHODS

Nowadays, composite materials are replacing metal materials, especially in the aviation industry. Carbon fiber composite materials are becoming increasingly popular due to their high strength-to-density ratio and high stiffness. In addition to the aviation industry, where strength-to-density and hardness ratios are of great importance, there are now vehicles produced entirely from carbon fiber in the maritime and automotive sectors. Boeing

787 Dreamliner and Airbus A350 are prime examples of next-generation aircraft made from carbon fiber materials.

Considering an isotropic substance in which heat transfer depends on temperature, the basic equation of heat transfer is as follows:

$$Q=\rho C\frac{\partial T}{\partial t}-\left(\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}\right)Q \tag{1}$$

where *qx* and *qy* (W/m^2) are the components of heat flow per surface area, (W/m^3) is the internal heat production rate per unit volume, ρ (kg/m^3) is the material density, (kJ/kg K^{-1}) is the heat capacity, *T* (K) is the temperature, and *t* (s) is the time. According to Fourier's law, the components of the heat flow can be written by substituting them into equation 1:

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+Q=\rho C\frac{\partial T}{\partial t}C \tag{2}$$

where *k* (W/m K^{-1}) is the heat conduction coefficient. In this study, it is assumed that there is no heat production ($Q=0$), the heat transfer is stable, that is, $dT/dt=0$, and there is also a constant boundary condition. Temperature is applied to one side of the RVE, and heat flux is applied to the other side. Considering that the RVE in question contains CCNT helical nanoparticles of the polyethylene nanocomposite, equation 3 is used to calculate the effective conduction coefficient of the RVE:[24]

$$k_{eef}^{\ast}\frac{T}{L}=q_{eff}q_i \tag{3}$$

where *T* (ΔK) is the temperature difference between the 2 surfaces of the RVE after analysis, *L* is the length of the RVE after analysis, and (W/m^2) is the equivalent flux passing between the 2 desired surfaces of the RVE. The effective heat flux value is obtained from the following relationship:

$$q_{ff}=\left(\sum_{i=1}^{N}q_i v_i\right)/V \tag{4}$$

Here, *V* (m^3) is the total volume of the RVE, the flux passing through each element, and the volume of each element, and *N* is the number of elements. It can also be said that thermal resistance is assumed in this study. The gap between the nanoparticles and the matrix is 0. It is explained in the next section that the element represents volume.

In this section, the RVE is restructured in two dimensions by scattering nanoparticles into it. Then, the optimum RVE size is obtained by determining the characteristics and mechanical and thermal properties of the matrix and nanoparticles. In this study, RVE was considered a two-dimensional cubic element. By using the Monte Carlo algorithm to distribute the CCNT nanoparticles in the mentioned RVE, the coordinates of the nanoparticles were first created in a text file with a MATLAB program. To calculate the orientation of nanoparticles, the angles of the global coordinate system of the longitudinal vector of nanoparticles are defined by the Monte Carlo algorithm in the following equation:[25]

$$\begin{cases}\theta=2\pi a\\ \varphi=cos^{-1}\left(2b-1\right)\end{cases} \tag{5}$$

In equation 5, θ and φ are the angles of the spherical coordinate device of the longitudinal vector of nanoparticles, as shown in Figure 1, and the coefficients *a* and *b* are 2 random numbers between 0 and 1. As an example of the distribution of CCNT nanoparticles in RVE with a volume percentage of 0.420%, the ratio of RVE length to CCNT is equal to 5.5 and 64 CCNT particles.

To make the RVE as a representative of the homogeneous volume of a heterogeneous material, after the optimal distribution of nanoparticles in it, its size also needs to be determined accurately; that is, the effective properties of the material do not depend on the size of the material. For this purpose, two different sizes of RVE with a volume percentage of 0.42% were created from nanoparticles of sizes 900 and 100 (with equal aspect ratio and volume percentage), according to Figure 2. Moreover, considering that the Monte Carlo algorithm is a random algorithm, each of the analyses was repeated 3 times, and the values presented in this study are the average of 3 heat transfer coefficients repeated so that the resulting value has less error. It is noteworthy that network growth is also used to increase the accuracy of the numerical solution and reduce the computational volume. Areas far from where the CCNT nanoparticles are located have a coarser network, but areas near the CCNT nanoparticles have a much finer network, with the total minimum number of RVE network elements being 500 000 and the number of CCNT nanoparticles being 50 000.

RESULTS AND DISCUSSION

The thermal conductivity coefficient was measured for both models, and according to the results reported in Figure 3, it can be seen that the responses for RVE at sizes 900 and 1000 are independent of the size of RVE.

The effects of different parameters, such as volume percentage of nanoparticles, their size, and diffusion direction, on the thermal

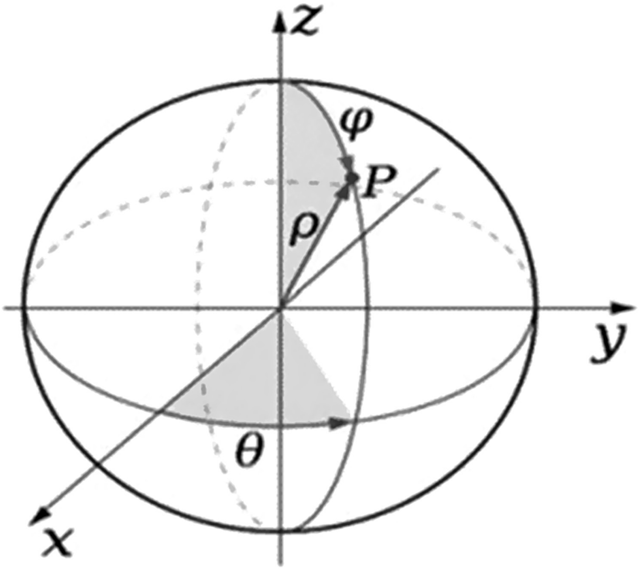

Figure 1. Spherical coordinates of the longitudinal vector of nanoparticles.[26]

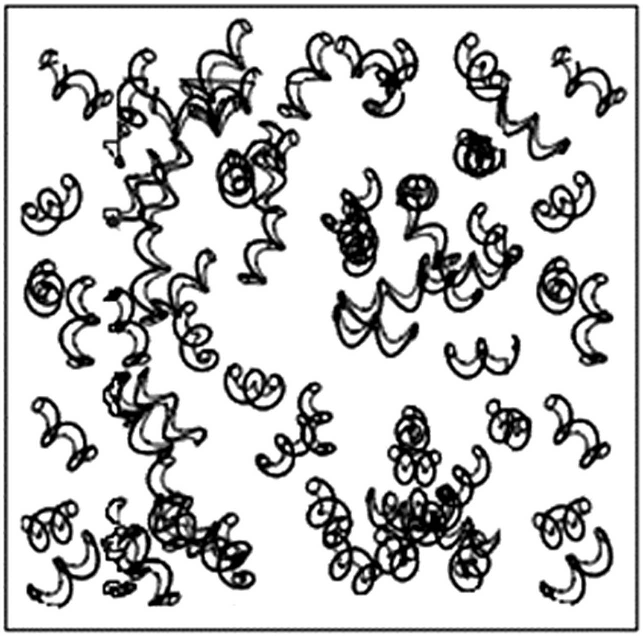

Figure 2. An example of the RVE structure containing 0.42% carbon nanotube by volume and the ratio of Representative Volume Elements (RVE) to carbon nanotube.

conductivity coefficient of the nanocomposite are discussed. The properties of nanoparticles are available in Table 1.

In order to observe the effect of the volume percentage of CCNT nanoparticles on the thermal conductivity coefficient of the nanocomposite, 4 different volume percentages of CCNT1-type CCNT nanoparticles were made, and then the resulting diagram of the finite element results was obtained as shown in Figure 4. As can be seen, the volume percentage of nanoparticles increased, and the amount of heat conduction coefficient increased continuously.

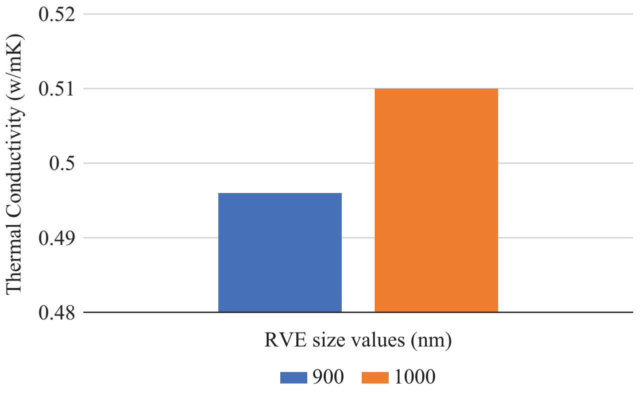

Figure 3. Thermal conduction coefficient graph of the nanocomposite for different RVE size values.

Table 1. Geometric Properties and Nomenclature of Nanoparticles

Type of Nanoparticles	Inner Diameter (nm)	Radius (nm)	Length (nm)
CCNT1	15	10	150
CCNT2	20	10	60-450
CCNT3	30-50	10	150
CCNT4	25	15	150

CCNT, carbon nanotube.

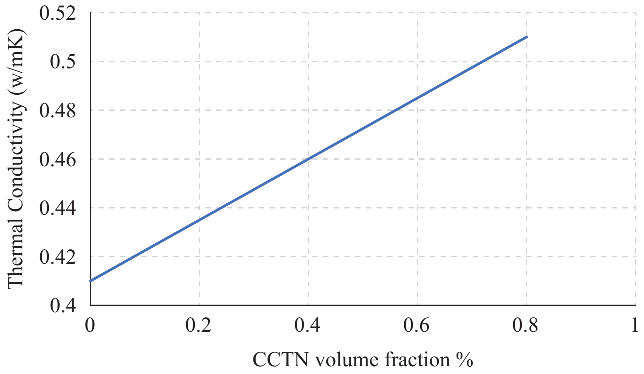

Figure 4. Graph of changes in thermal conductivity coefficient according to volume percentage of nanoparticles

The results obtained from studying the impact of various parameters on the thermal behavior of nanocomposites with CCNTs contribute to a better understanding of how these materials function and can be optimized for various applications. Here is how the results enhance our understanding:

Improved Material Design: Understanding how the volume percentage, aspect ratio, radius, and chirality of CCNTs affect thermal conductivity helps in designing nanocomposite materials with tailored thermal properties. This knowledge enables engineers and researchers to create materials with enhanced heat-transfer capabilities for specific applications, like thermal management in electronics.

Optimal Use of CCNTs: By knowing how these parameters influence thermal behavior, it becomes possible to optimize the use of CCNTs in composite materials. This can lead to more efficient and cost-effective solutions for improving heat dissipation in electronic devices, aerospace components, and other industries.

Insights into Phonon Behavior: The study of how defects and functionalization affect thermal properties sheds light on the role of phonons in heat conduction within CCNTs. This understanding can be used to control and manipulate phonon scattering, thereby enabling better control of thermal conductivity in nanocomposites.

Temperature-Dependent Behavior: Recognizing how temperature affects the thermal properties of CCNT-based nanocomposites is crucial for applications where materials operate under varying temperature conditions. This information can guide the design of materials that perform optimally at specific temperature ranges.

Practical Applications: The research results can lead to the development of advanced thermal interface materials, heat sinks, and other components that are essential for efficient heat management in electronic devices, advanced materials, and energy storage systems. This knowledge can result in more effective and durable products.

Sustainability and Energy Efficiency: Understanding how CCNT parameters impact thermal behavior can contribute to the development of materials that improve energy efficiency in various industries. This is particularly important for reducing energy consumption and carbon emissions in a range of applications. In conclusion, the results of studying the influence of parameters on the thermal behavior of nanocomposites with CCNTs provide valuable insights into material design and optimization, as well as a deeper understanding of phonon behavior and temperature-dependent characteristics. This knowledge can be harnessed to develop more efficient and sustainable materials for a variety of applications, ultimately contributing to advancements in technology and energy management.

In this study, the effect of adding nanoparticles of helical carbon tubes to polyethylene and obtaining the thermal properties (thermal conductivity coefficient) of the resulting nanocomposite was investigated. The research method was carried out with the help of a finite element numerical solution and also by dispersing the nanoparticles using the MATLAB program with the help of the Monte Carlo algorithm. After making the desired RVEs and performing thermal analyses on them, the results showed that the thermal conductivity coefficient increased with the increase of the volume percentage, arc length, and outer or inner radius of the nanoparticles. The thermal conductivity coefficient was obtained depending on the changes in the ratio of the free length of the CCNT to its diameter, and it was observed that the value increased as this ratio increased. It is different with the increase of each of these parameters so that the volume percentage parameter has the most effect on increasing the thermal conductivity coefficient of nanocomposite by 12.5%, and the external or internal diameter of nanoparticles and also the spring length of nanoparticles have the least effect on increasing the coefficient of conductivity.

The thermal conductivity of a nanotube is influenced by several parameters, including volume percentage, aspect ratio, radius, and more. Here is a concise summary of how each of these parameters can affect the thermal conductivity coefficient of nanotubes:

Volume Percentage
Higher volume percentages of nanotubes in a composite material generally lead to increased thermal conductivity. This is because a larger volume of nanotubes provides more pathways for heat conduction through the material.

Aspect Ratio
Nanotubes with higher aspect ratios (length-to-diameter ratio) tend to have better thermal conductivity. Longer nanotubes facilitate efficient phonon (vibrational heat carrier) transport, improving overall thermal conductivity.

Radius
The radius of a nanotube can influence its thermal properties. Nanotubes of smaller diameter may exhibit better thermal conductivity due to reduced phonon scattering, allowing heat to be conducted more efficiently.

Chirality
The chirality of a nanotube, which determines its atomic arrangement, can impact thermal conductivity. Some chiralities have inherently better thermal properties due to their electronic band structure, which affects phonon behavior.

Defects and Functionalization: The presence of defects or functional groups on the nanotube surface can hinder thermal conductivity by scattering phonons. However, controlled functionalization can be used to tune thermal properties for specific applications.

Temperature
Thermal conductivity often increases with rising temperature due to increased phonon mean free path. However, at extremely high temperatures, phonon–phonon scattering can reduce thermal conductivity.

Interactions with Surrounding Material: The thermal properties of nanotubes can be influenced by their interactions with the surrounding matrix material in composite systems. Strong nanotube–matrix interfaces can enhance thermal conductivity by promoting efficient heat transfer.

In summary, the thermal conductivity of nanotubes is influenced by a combination of intrinsic factors such as aspect ratio, radius, chirality, and defects, as well as extrinsic factors such as volume percentage and temperature. Understanding and manipulating these parameters is crucial for tailoring nanotube-based materials for specific thermal management applications.

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