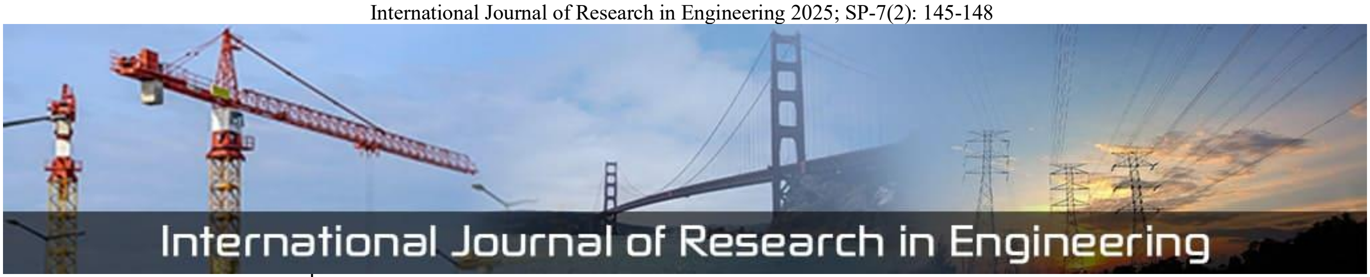

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Theoretical simulation on thermal conductivity of TiO_2 NPs and CNTs nanocomposite for thermal management

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Abstract
The demand for materials with enhanced thermal management capabilities is increasing, particularly in applications related to thermal comfort such as energy-efficient buildings, textiles, and electronic devices. This study investigates the thermal conductivity of titanium dioxide (TiO_2) and carbon nanotube (CNT) nanocomposites through numerical simulation. TiO_2 nanoparticles were synthesized via a green synthesis route using plant extracts, offering a sustainable and eco-friendly approach. Commercially obtained multi-walled CNTs were incorporated into the TiO_2 matrix at varying concentrations (0.9-0.01 wt%) to form nanocomposites. The effect of CNT loading on the effective thermal conductivity was analyzed using computational modeling techniques. The simulation results demonstrate a significant change in thermal conductivity with increasing CNT concentration, attributed to the low intrinsic thermal conductivity of CNTs and their synergistic interaction with the TiO_2 matrix. The findings suggest that TiO_2-CNT nanocomposites hold strong potential for use in thermal comfort applications where improved heat dissipation and thermal regulation are required.

Keywords: Titanium dioxide NPs, carbon nanotubes, nano composite, thermal conductivity

Introduction

In recent years, the pursuit of advanced materials with enhanced thermal management capabilities has gained significant attention, particularly in the context of improving thermal comfort in built environments, wearable technologies, and electronic devices [1-3]. Nanocomposites, formed by embedding nanoscale fillers into a base matrix, offer a promising route to tailor thermal conductivity and meet specific performance requirements. Among various nanomaterials, titanium dioxide (TiO_2) and carbon nanotubes (CNTs) stand out due to their unique thermal, mechanical, and structural properties.

TiO_2, a widely used metal oxide, exhibits moderate thermal conductivity, high thermal stability, and excellent chemical resistance [4]. On the other hand, CNTs possess extraordinarily high thermal conductivity, often exceeding 3000 W/m·K for individual tubes, making them ideal candidates for enhancing the thermal transport properties of composite materials [5-6]. The synergy between TiO_2 and CNTs in a nanocomposite structure presents a compelling opportunity to engineer materials that combine the advantages of both constituents-mechanical integrity from TiO_2 and superior thermal conductivity from CNTs.

Simulation studies play a crucial role in understanding the heat transfer behavior in such nanocomposites, allowing for the prediction and optimization of thermal conductivity without the need for extensive experimental trials. By employing computational models, such as finite element analysis (FEA) or molecular dynamics (MD), researchers can analyze the effects of parameters like filler concentration, dispersion, and interfacial thermal resistance on overall thermal performance.

This study aims to investigate the effective thermal conductivity of TiO_2-CNT nanocomposites through numerical simulations, focusing on their potential use in thermal comfort applications. By examining how the incorporation of CNTs influences heat conduction within the TiO_2 matrix, the research seeks to provide insights into material design strategies for energy-efficient and thermally comfortable solutions.

Experimental detail

Synthesis of TiO_2-CNT Nanocomposites

Green Synthesis of TiO_2 Nanoparticles

Titanium dioxide (TiO_2) nanoparticles were synthesized using a green synthesis approach, which is environmentally friendly and avoids the use of toxic chemical reagents. A plant extract (e.g., *Azadirachta indica*, *Moringa oleifera*, or another commonly used reducing agent) was prepared by washing fresh leaves thoroughly with distilled water, drying them at room temperature, and then boiling them in distilled water for 20-30 minutes. The extract was filtered and used as a reducing and stabilizing agent.

Titanium precursor, typically titanium (IV) isopropoxide (TTIP), was slowly added to the plant extract under constant stirring at room temperature. The reaction mixture was maintained under continuous stirring for several hours until a white precipitate began to form, indicating the formation of TiO_2 nanoparticles. The precipitate was collected by centrifugation, washed repeatedly with distilled water and ethanol to remove impurities, and then dried in a hot air oven at 80 °C. The dried powder was calcined at 450-500 °C for 2 hours to enhance crystallinity.

Preparation of TiO_2-CNT Nanocomposites

Commercially available multi-walled carbon nanotubes (MWCNTs) were used without further functionalization. To prepare the nanocomposites, TiO_2 nanoparticles were uniformly mixed with varying weight percentages of CNTs (e.g., 0.5 wt%, 1 wt%, 2 wt%, and 3 wt%) to study the effect of CNT concentration on thermal conductivity.

The required amount of CNTs was dispersed in ethanol by ultrasonication for 30 minutes to ensure proper deagglomeration. The TiO_2 nanoparticles were then added to the CNT dispersion and the mixture was further ultrasonicated for 1 hour followed by magnetic stirring for several hours to ensure homogeneous mixing. The resulting slurry was dried at 80 °C and then ground into fine powder for further analysis and characterization.

Results and Discussion

Scanning Electron Microscope

Characterization of TiO_2 nanoparticles (TiO_2 NPs) by Scanning Electron Microscopy (SEM) provides crucial insights into their surface morphology, particle size, shape, and agglomeration state [7-9]. SEM uses a focused beam of electrons to produce high-resolution images of the nanoparticle surface, allowing for detailed analysis at the nanometer scale. As shown in figure 1, SEM micrograph, TiO_2 nanoparticles typically appear as nearly spherical or irregularly shaped particles, often showing some degree of agglomeration due to their high surface energy. The surface texture and distribution can also be observed, giving clues about the synthesis method and uniformity of the particles. By using image analysis software in conjunction with SEM images, approximate particle size and size distribution can be determined.

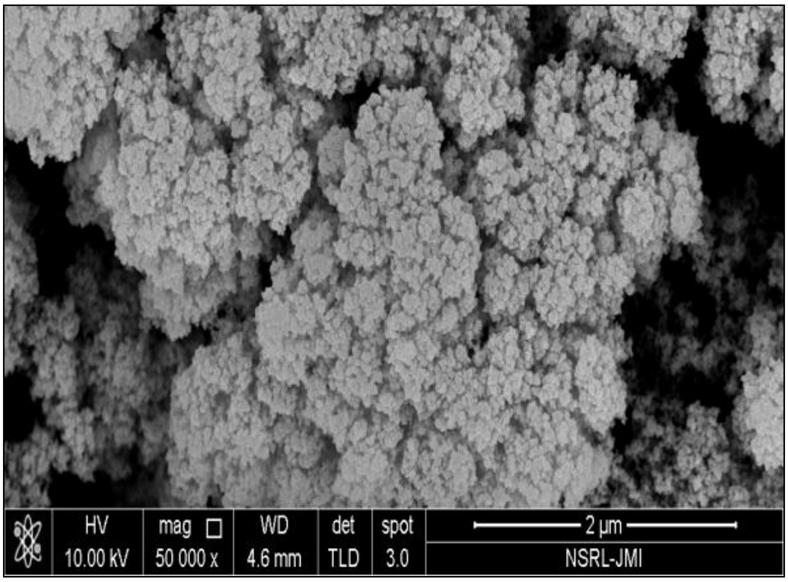

Fig 1: SEM micrograph of TiO2 NPs grown by Green method

Theoretical simulation of Thermal Conductivity of TiO_2 Nanoparticles

The study of the thermal conductivity of titanium dioxide (TiO_2) nanoparticles is essential for evaluating their potential in thermal insulation, photocatalysis, and electronic applications [10-12]. TiO_2 exists in various crystal forms-anatase, rutile, and brookite-each exhibiting different thermal transport properties due to variations in crystal structure, phonon scattering, and defect concentration [13-15]. At the nanoscale, the thermal conductivity of TiO_2 is significantly affected by particle size, shape, crystallinity, and agglomeration, as well as the surrounding medium when dispersed in fluids [16].

In this work, anatase TiO_2 has a thermal conductivity of approximately 3-5 W/m•K. it is well known that the material is reduced to the nanoscale, the thermal conductivity drops considerably due to increased phonon boundary scattering. This phenomenon limits the mean free path of heat-carrying phonons, especially in particles below 100 nm.

To estimate the effective thermal conductivity (k_{eff}) of TiO_2 nanoparticles dispersed in a fluid (i.e., in nanofluid applications), one commonly used model is Maxwell's Effective Medium theory [17-20], given by:

$$\mathbf{keff = kf \cdot \frac{kp + 2kf + 2\phi(kp - kf)}{kp + 2kf - \phi(kp - kf)}} \quad (1)$$

Where:

- k_{eff}: *Effective thermal conductivity of the nanofluid*
- k_p : *Thermal conductivity of the* TiO_2 *nanoparticles (8.4)*
- k_p: *Thermal conductivity of the base fluid (e.g., CNT (0.9)*
- ϕ: *Volume fraction of nanoparticles (0.9 to 0.01)*

This model assumes spherical particles and low concentrations ($\phi<0.1$). It shows that increasing the particle volume fraction or using nanoparticles with higher intrinsic thermal conductivity improves overall heat transfer. However, experimental studies often report deviations from this model, especially at higher concentrations or with agglomerated particles, due to additional effects such as Brownian motion, interfacial thermal resistance, and particle clustering.

In the present study, we theoretically investigate the thermal conductivity of TiO_2 nanoparticles (NPs) and their nanocomposites using Maxwell's equationas given in equation (1). Bare TiO_2 and TiO_2 NPs were dispersed with carbon nanotubes (CNTs) at varying volume concentrations ranging from 0.01% to 0.9%. Theoretical values were obtained using Python implementations of the Maxwell model, yielding thermal conductivity values for the TiO_2 nanocomposites in the range of 8.4 to 0.920 W/m·K.

The table (1) presents the thermal conductivity values of TiO_2 nanoparticles and their nanocomposites obtained by simulation. It is evident from the data that the nanocomposites exhibit lower k-values compared to bare TiO_2 NPs. This suggests that the nanocomposites offer improved thermal insulation properties, making them a promising approach for managing thermal behavior in everyday household appliances.

Table 1: Variation of thermal conductivity with different concentration of CNTs

S. No.	Nanocomposites	Thermal conductivity (k)
1	Bare TiO2 NPs	8.4
2	TiO2@CNT (0.9%)	6.183
3	TiO2@CNT (0.75%)	4.22
4	TiO2@CNT (0.5%)	2.472
5	TiO2@CNT (0.25%)	1.5
6	TiO2@CNT (0.1%)	1.11
7	TiO2@CNT (0.05%)	1.003
8	TiO2@CNT (0.02%)	0.942
9	TiO2@CNT (0.01%)	0.920

The variation in k-values from TiO_2 nanoparticles to their nanocomposites (as concentration of CNTs decrease) is significantly low, indicating a substantial improvement in thermal performance. This suggests that nanocomposites are highly effective for thermal management applications. In building materials, such nanocomposites can help regulate indoor temperatures by enhancing insulation, thereby reducing energy consumption for heating or cooling. Their superior thermal properties make them ideal candidates for future use in sustainable construction and energy-efficient home appliances. As the demand for advanced thermal insulation materials grows, TiO_2-based nanocomposites offer a promising solution for both environmental and economic benefits in various practical applications.

Conclusion

This study demonstrates the potential of TiO_2 nanocomposites for effective thermal management in building applications. Theoretical calculations based on Maxwell's model revealed that the thermal conductivity of TiO_2 nanocomposites decreases with the incorporation of carbon nanotubes, ranging from 8.4 to 0.920 W/m·K depending on the CNT concentration. The simulated k-values for the nanocomposites were significantly lower than those of bare TiO_2 NPs, indicating improved thermal insulation performance. These findings suggest that TiO_2-based nanocomposites are promising materials for controlling heat flow in buildings, contributing to energy efficiency and sustainable construction practices in future infrastructure development.

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