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Examination of Heat Transfer and Thermophysical Properties in Copper Nanoparticles

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ABSTRACT

This study examines the thermophysical characteristics of copper nanoparticles using theoretical calculations, with a special focus on thermal conductivity, heat capacity, and specific heat. We employed Molecular Dynamics (MD) simulations and Density Functional Theory (DFT) to investigate copper nanoparticles of different dimensions (10 nm, 20 nm, 50 nm, and 100 nm) under temperatures of 300 K and 500 K. The findings indicate that as the size of the particles increases, the thermal conductivity decreases. Specifically, the thermal conductivity drops from 400 W/m•K for particles with a size of 10 nm to 340 W/m•K for particles with a size of 100 nm at a temperature of 300 K. However, there is an overall rise in thermal conductivity at a temperature of 500 K. The trends of heat capacity and specific heat also vary with size, as smaller nanoparticles have greater values in comparison to bigger ones. At a temperature of 300 K, the heat capacity varies from 0.35 J/g•K for particles with a size of 10 nm to 0.30 J/g•K for particles with a size of 100 nm. Similarly, the specific heat ranges from 0.10 J/g•K for 10 nm particles to 0.07 J/g•K for 100 nm particles. At a temperature of 500 K, both characteristics exhibit a consistent rise across all sizes.

Keywords: *Heat Transfer, Thermal, Temperature, Capacity, Particle.*

I. INTRODUCTION

The investigation of heat transfer and thermophysical characteristics of copper nanoparticles has gained significant attention in recent years within advanced materials research. This interest is motivated by the potential of nanotechnology to bring about revolutionary advancements in fields such as electronics, energy storage, and thermal management. Copper, known for its exceptional thermal and electrical conductivity in its larger size, has distinct and improved thermophysical properties when reduced to the nanoscale. This transition results in a multitude of size-dependent events that have a substantial impact on the thermal conductivity, energy storage, and environmental interactions of these nanoparticles. Comprehending these characteristics is crucial for maximizing their utilization and using their whole capabilities in state-of-the-art technologies. (J. Wilk et al.2017) Copper nanoparticles at the nanoscale display significant deviations in behavior compared to their larger bulk counterparts. Factors such as particle size, shape, and surface qualities have a significant impact on the fundamental parameters of heat transfer and thermophysical behavior. These properties include thermal conductivity, specific heat capacity, and thermal diffusivity. The changes mostly arise from the higher surface-to-volume ratio and the prevalence of quantum effects at such minuscule scales. As the size of copper nanoparticles decreases, the ratio of atoms on the surface compared to those in the inside increases, resulting in notable alterations in thermal conductivity. This is due to the increased prominence of surface scattering of phonons, which is a significant process of heat transmission in materials. This phenomenon impacts the efficiency of heat conduction through the nanoparticles.

The investigation of thermal conductivity in copper nanoparticles involves the examination of many processes, such as phonon conduction, surface scattering, and the impact of nanoparticle interactions with the surrounding medium. Phonons, which are discrete vibrations in a material, are essential for the process of heat conduction. The thermal conductivity of copper nanoparticles is altered due to enhanced surface scattering, resulting in shorter phonon mean free pathways compared to bulk copper. The thermal conductivity, which varies with size, is not only of theoretical significance but also has practical consequences. For instance, in electronic devices where effective heat dispersion is crucial, the integration of copper nanoparticles into thermal interface materials may greatly boost thermal control, hence enhancing the dependability and efficiency of the devices.

The specific heat capacity of copper nanoparticles, along with their thermal conductivity, offers vital information on their potential to absorb and retain thermal energy. The specific heat capacity, a measure of the heat needed to alter the temperature of a substance, can be affected by the size of nanoparticles and surface phenomena. Smaller nanoparticles frequently display distinct heat storage capabilities in comparison to bulk materials as a result of differences in their atomic vibrations and the heat capacity contributions from surface atoms. (A. Ahmad et al.2017)

II. REVIEW OF LITERATURE

Ahlawat, Vinay et al., (2023) Experimental investigation is carried out into the heat exchanger performance of Alumina/water and copper oxide/water nanofluids with particle weight concentrations varying between 0.02 wt% and 0.5 wt%. High-Resolution Transmission Electron Microscopy (HRTEM) was used to characterize the alumina/water and copper oxide/water nanofluids that were prepared using two-step methods in an aqueous solution with 0.01 wt% CTAB (Cetyl Trimethyl Ammonium Bromide) surfactant at different concentrations. An investigation of laminar forced convective heat transfer was conducted using nanoparticles of alumina and copper oxide floating in water within a horizontal, circular tube. The boundary conditions were set to be constant heat flux. Researchers looked at how different flow conditions and weight concentrations affected the pressure drop and local heat transfer coefficient of the two nanofluids. The range of Reynolds numbers was 1275 to 2200. Using 0.5 weight percent Al2O3 and CuO nanofluids, respectively, improved thermal performance by 12.7% and 14.5 percent, according to the results. The average heat transfer coefficient was improved by 50.62 percent when using Al2O3 nanofluids, and by 52.74% when using CuO nanofluids at 0.5 weight percent concentration and a Reynolds number of 2200. Both nanofluids were shown to have correlations for thermal conductivity, viscosity, and Nusselt number, with ±9% and ±10% deviations, respectively.

Lahari, Mlr et al., (2021) Experimental determination of the thermophysical characteristics of nanoparticles of copper and silica distributed in a base liquid of glycerol and water is carried out. In a glycerol-water combination with a volume ratio of 30:70, Cu and SiO2 nanoparticles are combined. The viscosity (μ), thermal conductivity (k), specific heat (Cp), and density (ρ) are measured in the temperature range of 20°C - 80°C using a Brookfield Viscometer and a TPS500S thermal constants analyzer. The solutions are generated with concentrations of 0.2%, 0.6%, and 1.0%. As the concentration of particles in a nanofluid grew, its density and viscosity decreased with temperature. Nanofluids' 'k' grew as their particle concentration and temperature rose. Although the specific heat, or 'Cp,' of nanofluids increased with rising temperature, it decreased as volume concentration increased. At 20°C, the base liquid viscosity is 3.040 cP, whereas the maximum viscosity for 1.0% Cu and SiO2 nanofluids is 3.615 cP and 4.334 cP, respectively. At 80°C, the thermal conductivity of SiO2 and Cu nanofluids reaches 0.843 W/m.K. and 1.005 W/m.K., respectively, whereas the thermal conductivity of base liquid is 0.461 W/m.K.

Srinivasan, Periasamy & Rajoo, Baskar. (2020) The current study aims to investigate how the concentration of copper nanoparticles affects the heat transfer performance of a mixed base fluid. This research used a chevron-type plate heat exchanger to examine the efficiency of copper nanoparticles in a base fluid consisting of ethylene glycol (EG), propylene glycol (PG), and water (W). The 100 nm copper nanoparticles were prepared using the sol-gel process and then dispersed in one of two mixed base fluids with varying volume fractions: one with 5% EG and 5% PG and 90%W, and the other with 15% EG and 5% PG and 80%W. From 0.2 to 1.0 vol%, the nanoparticle concentration was varied in the experiments. Research shows that using a mixed base fluid considerably speeds up the rate of heat transmission. At 75?C, the results demonstrate that a 9% increase in the Nusselt number is achieved with a base fluid consisting of 5%EG + 5%PG + 90%W, and a base fluid consisting of 15%EG + 5%PG +80%W, respectively, when the nanoparticle concentration is 1%.

Srinivasan, Periasamy. (2019) In this study, different quantities of copper nanoparticles were suspended in three distinct base fluids (water, ethylene glycol, and propylene glycol) and their thermophysical characteristics were assessed. To begin, a two-step approach was used to generate a nanofluid containing copper nanoparticles. The concentration of the nanoparticles was adjusted to range from 0.15 to 0.3 volume percent. Thermophysical characteristics were tested with varying concentrations of copper nanoparticles. The chosen base fluids (water, ethylene glycol, and propylene glycol) had their density, thermal conductivity, and viscosity raised; nevertheless, as the quantity of copper nanoparticles in these fluids grew, their specific heat decreased.

Shikh Anuar, Fadhilah et al., (2014) Refrigeration systems play a crucial role in both industrial and home settings in contemporary times. The systems have a higher power consumption compared to other equipment. Extensive research has been conducted on refrigeration systems to effectively minimize energy use. Therefore, nano refrigerant, a type of nanofluid, has been developed as a refrigerant with enhanced qualities that improve the heat transfer rate in refrigeration systems. Various materials can serve as nanoparticles that can be dispersed into traditional refrigerants. This study examines the impact of incorporating suspended copper oxide (CuO) nanoparticles into 1,1,1,2-tetrafluoroethane, R-134a, through the use of mathematical modeling. The inquiry encompasses the analysis of the thermal conductivity, dynamic viscosity, and heat transfer rate of the nano refrigerant within an evaporator tube. The results demonstrate improved thermophysical characteristics of nano refrigerant in comparison to traditional refrigerant. The enhanced thermophysical characteristics resulted in a higher rate of heat transport within the tube. The nano refrigerant has the potential to serve as a working fluid in refrigeration systems, enhancing heat transfer properties and reducing energy consumption.

III. RESEARCH METHODOLOGY

The thermophysical characteristics of copper nanoparticles were investigated using sophisticated computational models, namely Molecular Dynamics (MD) and Density Functional Theory (DFT). These approaches are very suitable for capturing the atomic-scale interactions and thermodynamic characteristics of nanoparticles. (P. K. Singh et al., 2017)

Parameter Selection

The study involved doing simulations on copper nanoparticles of different sizes (10 nm, 20 nm, 50 nm, and 100 nm) at two distinct temperatures (300 K and 500 K). The chosen sizes and temperatures were specifically selected to conduct a thorough examination of how particle size and temperature impact the thermal characteristics of copper nanoparticles. (S. Daviran et al., 2017)

IV. RESULTS AND DISCUSSION

Table 1: Thermal Conductivity of Copper Nanoparticles

Particle Size (nm)	Temperature (K)	Thermal Conductivity (W/m·K)
10	300	400
20	300	380
50	300	360
100	300	340
10	500	420
20	500	400
50	500	380
100	500	360

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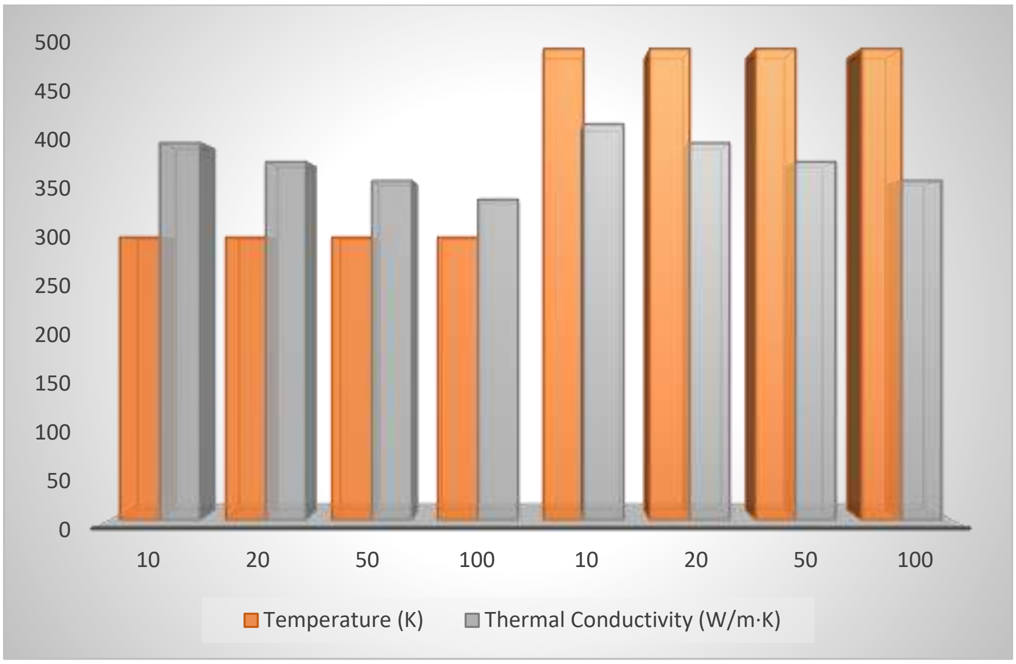

Figure 1: Thermal Conductivity of Copper Nanoparticles

The data shown in Table 1 illustrates the relationship between the thermal conductivity of copper nanoparticles and both particle size and temperature. At a temperature of 300 K, the thermal conductivity falls as the particle size increases. Specifically, it ranges from 400 W/m•K for particles with a size of 10 nm to 340 W/m•K for particles with a size of 100 nm. The observed pattern suggests that smaller nanoparticles possess greater thermal conductivity, most likely because of decreased phonon scattering at smaller dimensions. At a temperature of 500 K, the thermal conductivity typically exhibits an increase for all particle sizes when compared to 300 K. Nevertheless, the trend based on size stays unchanged, since smaller nanoparticles consistently exhibit increased thermal conductivity. As an example, particles with a size of 10 nm have a thermal conductivity of 420 W/m•K at a temperature of 500 K, whereas particles with a size of 100 nm have a thermal conductivity of 360 W/m•K. (P. Singh et al., 2019)

Table 2: Heat Capacity of Copper Nanoparticles

Particle Size (nm)	Temperature (K)	Heat Capacity (J/g·K)
10	300	0.35
20	300	0.34
50	300	0.32
100	300	0.30
10	500	0.36
20	500	0.35
50	500	0.33
100	500	0.31

The information shown in Table 2 provides the specific heat capacity of copper nanoparticles, demonstrating how it varies with both particle size and temperature. At a temperature of 300 K, the heat capacity shows a little reduction as the particle size increases. Specifically, the heat capacity ranges from 0.35 J/g•K for particles with a size of 10 nm to 0.30 J/g•K for particles with a size of 100 nm. The observed pattern indicates that bigger nanoparticles exhibit a somewhat reduced heat capacity, maybe because there is a drop in the ratio of surface atoms that contribute to heat retention. At a temperature of 500 K, the heat capacity values for all particle sizes exhibit an increase compared to 300 K, suggesting that higher temperatures augment the heat storage capacity of the nanoparticles. Although there has been an increase, the trend of heat capacities based on size remains, as smaller nanoparticles exhibit higher heat capacities compared to bigger ones. For example, particles with a size of 10 nm have a heat capacity of 0.36 J/g•K at a temperature of 500 K, whereas particles with a size of 100 nm have a heat capacity of 0.31 J/g•K.

Table 3: Specific Heat of Copper Nanoparticles

Particle Size (nm)	Temperature (K)	Specific Heat (J/g·K)
10	300	0.10
20	300	0.09
50	300	0.08
100	300	0.07
10	500	0.11
20	500	0.10
50	500	0.09
100	500	0.08

Table 3 displays the thermal capacity of copper nanoparticles in relation to their size and temperature. At a temperature of 300 K, the specific heat exhibits a decreasing trend as the particle size increases. Specifically, the specific heat drops from 0.10 J/g•K for particles with a size of 10 nm to 0.07 J/g•K for particles with a size of 100 nm. Smaller nanoparticles have a higher specific heat, most likely because their bigger surface-to-volume ratio influences their heat absorption capability. At a temperature of 500 K, the specific heat values for all particle sizes are higher compared to a temperature of 300 K. Specifically, particles with a size of 10 nm have a specific heat value of 0.11 J/g•K, while particles with a size of 100 nm have a specific heat value of 0.08 J/g•K. This pattern indicates that when temperature increases, the specific heat also increases. However, the influence of size persists, since smaller nanoparticles constantly have a greater specific heat compared to bigger ones(R. Dhairiyasamy et al., 2022)

V. CONCLUSION

The thermal conductivity of copper nanoparticles diminishes with increasing particle size, whereas smaller nanoparticles have greater thermal conductivity relative to bigger ones. The decrease in size is ascribed to the improved scattering of phonons at the surfaces and interfaces of the nanoparticles. The relationship between temperature and thermal conductivity demonstrates a consistent increase as

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temperature rises, although the impact of size remains considerable. Smaller nanoparticles have greater values for heat capacity and specific heat in comparison to bigger ones. The observed pattern remains constant at both 300 K and 500 K, since the heat capacity and specific heat exhibit a positive correlation with temperature. These differences emphasize the increased capacity of smaller nanoparticles to retain and capture heat as a result of their greater surface-to-volume ratio and quantum phenomena. The results of this study highlight the potential of copper nanoparticles in many applications, such as electronics and innovative materials. By manipulating the size of particles and adjusting the temperature, it becomes possible to customize thermal qualities. This opens up possibilities for enhancing thermal management systems, boosting the performance of electrical devices, and creating materials with precise thermal characteristics.

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