CHAPTER 1 Introduction

1.1. Background

Heat transfer fluids play a vital role in different industrial sectors and sophisticated components. However, conventional heat transfer fluids, such as water, ethylene glycol, oil, etc. are not suitable in all of these applications. The poor heat transfer capability of these common fluids is a primary impediment to the effectiveness of heat exchangers. Several attempts have been made by scientists and engineers to improve the heat transfer efficiency of the conventional fluids. It is well known that metal in solid form have higher thermal conductivities than those of fluids. For example, the thermal conductivity of Cu at room temperature is 700 times greater than that of water and 3000 times greater than that of engine oil. Because of the fact that solids have thermal conductivities a few orders of magnitude higher than liquids, different slurries have been produced by suspending millimeter or micrometer-sized particles in the conventional heat transfer fluids (Ahuja, 1975). However, the heat transfer enhancement of the slurries is not up to the requirement of advanced heat transfer applications. Moreover, it causes some problems in the applications, such as, clogging, sedimentation, erosion, increase in pressure drop, etc. Therefore, slurries can not be used effectively as the replacement of conventional heat transfer fluids in modern energy efficient and sophisticated instruments. Based on the fact that heat transfer in suspensions takes place through the interface between the dispersoids and liquid, researchers have tried to enhance the heat transfer rate by using dispersoids with higher surface area-to-volume ratio, i.e., by using particles with reduced size. Modern nanotechnology has enabled to produce particles with size less than 100 nm having surface area-to-volume ratio several orders of magnitude larger than millimeter or micrometer-sized particles. Thus, recognizing an opportunity to apply this emerging nanotechnology to the established thermal engineering, Choi (1995) proposed that nanoparticles could be suspended in industrial heat transfer fluids to produce a new class of engineered fluid (called nanofluid) with high thermal conductivity. Nanofluids are attractive heat transfer media as their thermal conductivities are significantly higher than those of parent liquids even when the volume fraction of nanoparticles is negligible (Choi, 1995; Eastman *et al.*, 2001; Lee *et al.*, 1999). The problems encountered with the use of common slurries as heat transfer media are mostly absent with nanofluids, which makes it suitable in modern miniaturization technology.

Diverse types of nanofluids have been produced and characterized since the last decade by different investigators. The enhancement in thermal conductivity of nanofluids is found to depend on the type of nanoparticles and base fluid, volume fraction of nanoparticles, temperature of the liquid medium, size and shape of the nanoparticles, type of dispersant used for stabilization, etc. Eastman *et al.* (2001) have experimentally investigated the thermal conductivity of ethylene glycol (EG) based Cu (<10 nm dia.) nanofluid and have found the enhancement in thermal conductivity of 40% over the base fluid for a volume fraction of 0.3% Cu nanoparticle. Lee *et al.* (1999) have carried out study on water and ethylene glycol based Al_2O_3 and CuO nanofluids and have observed significant enhancement in thermal conductivity depending on the type of nanoparticle and base fluid and/or size of the nanoparticle. The temperature dependence of thermal conductivity enhancement of water based Al_2O_3 and CuO have been experimentally investigated by Das *et al.* (2003), who observed 2 to 4 fold increase in thermal conductivity enhancement of the nanofluids over a temperature range of 21 to 51°C. Murshed *et al.* (2005) have carried out study on water based nanofluids containing TiO_2 nanoparticles of two different shapes. They have expressed that apart from particle size, the shape of the particle also has an influence on the thermal conductivity enhancement of nanofluids. The experimental investigation by Patel *et al.* (2003) on the thermal conductivity of water and toluene based nanofluids containing Au and Ag particles points out the positive role of dispersant to improve the enhancement.

Theoretical investigation on the thermal conductivity enhancement of nanofluids is limited. Although some discrete attempts have been made by some researchers to model the heat transfer of nanofluids, a universally accepted model still does not exist. The mechanism of heat transfer of nanofluids has not been established as yet. Conventional continuum models, such as Maxwell's model (Maxwell, 1904), Hamilton and Crosser's model (Hamilton and Crosser, 1962), etc. underpredict the thermal conductivity enhancement of nanofluids to a great extent. Keblinski *et al.* (2002) have explored four possible explanations for the enhanced thermal conductivity of nanofluids, such as Brownian motion of nanoparticles in the nanofluid, ordered layering of liquid molecules at the liquid/particle interface, ballistic nature of heat transport in the nanoparticles, and nanoparticles clustering effect. However, none of these mechanisms could provide a complete rational explanation to the enhanced thermal conductivity observed in nanofluids. Although the existing models based on the assumption of Brownian motion (Shukla and Dhir, 2005; Bhattacharya *et al.*, 2004), microconvection associated with Brownian motion (Jang and Choi, 2004; Prasher *et al.*, 2006a), interfacial nanolayering (Leong *et al.*, 2006), nanoparticles aggregation (Prasher *et al.*, 2006b), etc. could predict the thermal conductivity enhancement for some specific systems, a generalized model having the capability to explain the enhanced thermal conductivity of the diverse types of nanofluids is yet to emerge. Thus, designing the nanofluids for practical applications is still a real problem.

1.2. Motivation for the Present Study

Although some attempts have been made to model the thermal behavior of nanofluids, the observed enhancement in thermal conductivity of nanofluids is still a question of debate. It has been suggested by several authors (Keblinski *et al.*, 2002; Timofeeva *et al.*, 2007; Nie *et al.*, 2008; Evans *et al.*, 2006) that the contribution of Brownian motion and its micro-convection effect are negligible in carrying the heat through the nanofluid because of the fact that Brownian motion velocity and convection current velocity is smaller than the normal diffusive heat transport into the base fluid. However, heat transfer due to collision of the particles with the heat source has not been focused on. The present simulations based on classical molecular dynamics (MD) have shown that during collision of a nanoparticle with a heat source a pulse-like heat transfer occurs. This phenomenon has, however, been overlooked in all the existing models of nanofluids. The present study has attempted to explore the contribution of this collision induced heat transfer to the enhanced thermal conductivity of nanofluids. The nanoparticles inevitably move in the nanofluid by Brownian motion due to their small size and eventually collide with the heat source at a certain frequency depending on the Brownian motion parameters. From Brownian dynamics, collision frequency can be estimated. The Brownian motion of nanoparticles suspended in a nanofluid and the associated thermal evolution can be tracked with the help of stochastic simulation. By combining MD model with stochastic model, it is possible to evaluate the thermal characteristics of nanofluids. The present work explores this possibility to theoretically estimate the thermal conductivity of diverse types of nanofluids in order to design nanofluids for practical applications.

1.3. Objectives of the Present Research

The objectives of the present study are as follows:

a) To simulate the heat transfer associated with the collision of a Cu nanoparticle with a Cu heat source by MD simulation technique.
b) To simulate the Brownian motion of the Cu nanoparticle in water medium and the associated thermal evolution of the nanoparticle, by stochastic simulation.
c) To estimate the enhancement in thermal conductivity of the water based Cu-nanofluid for a given volume fraction loading of nanoparticles, on the basis of the thermal history of the suspended nanoparticles in the base fluid (water).
d) To perform the coupled MD-stochastic simulation to evaluate the effect of the material, size and shape of the nanoparticle, and temperature of the base fluid on the thermal conductivity of nanofluids.
e) To synthesize different types of nanofluid and characterize them with an aim to validate the prediction of the theoretical model.
f) To establish applicability of the model to diverse types of nanofluids and thus assessing its reliability.
g) To develop a highly conductive nanofluid suitable for the advanced heat transfer applications with the help of the information obtained from the coupled MD-stochastic model of heat transfer of different types nanofluids.