

A MOLECULAR DYNAMICS STUDY ON VISCOUS AND THERMAL PROPERTIES OF NANOFUIDS

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Thesis submitted in partial fulfillment of the requirements for the degree Master of
Science

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March 2023

Declaration

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To My Loving Parents, My Sister, My Brother, and My Late Friend, Dilash

Acknowledgments

It should be mentioned first, that I have been blessed with peerless support from my main supervisor, Dr. Nalaka Samaraweera over the past two years at the University of Moratuwa. His broad knowledge on the subject and critical thinking, greatly helped me to shape this work to its current form. The freedom and independence he gave me, guide me toward a better researcher. I am truly grateful to him for making this journey possible. I also do express my gratitude to my co-supervisors, Dr. Saliya Jayasekara and Prof. Kapila Perera, for their kind support during my studies. They were always ready to help me providing their expertise on the subject. I greatly appreciate the contribution given by my supervisors for the successful completion of this work.

My interest towards scientific research was initially identified by Dr. Anusha Wijewardane and she guided me towards my dreams from the scratch. She saw the potential in me and believed in me at times that were not easy for me. There won't be enough words in any of the languages that exist to express how I am grateful to her. So, I would just say "Thank You". I also want to appreciate the support given by Dr. Chathura Ranasinghe via allocating his computational resources to my work. The tremendous support given by my good friend, Pasan Henadeera, should be appreciated as well. From sharing his personal computational resources to the insightful comments he gave me on the subject matter, helped me for the successful completion of this work.

The support given by technical officer Mr. K.T. Priyantha and lab attendant Mr. U.W.T.N. Piyawardana at the Aeronautical Lab, Department of Mechanical Engineering, University of Moratuwa should be acknowledged. I am also grateful for the support given by Mr. N.A.D.K.A. Jayawardana, the system analyst at the Department of Mechanical Engineering, University of Moratuwa by upkeeping the workstation computers even during the pandemic times. Sincere thanks go to all of the members of the Department of Mechanical Engineering, University of Moratuwa as well for their support. The financial assistance provided by the Senate Research Grant (SRC/LT/2020/15), University of Moratuwa should also be acknowledged.

Last but not least, I would like to thank my father, mother, sister, and to my brother for their selfless dedication to creating a peaceful working environment for me. Their tremendous support is highly appreciated and will be remembered forever.

The aim of this study is to understand the microscopic behavior of heat and momentum transfer in nanofluids. With nanofluids reporting enhanced thermal conductivities (κ) and viscosities (η), a microscopic understanding is essential for engineering nanofluids to be practical in heat transfer applications. Therefore, to study the microscopic transport behavior, copper-argon nanofluids simulated by classical molecular dynamics are employed. The Applicability of the Green-Kubo (GK) method in nanofluid κ evaluation is questioned as the calculated thermal conductivities through the GK method are considerably higher than the direct method in Non-Equilibrium-Molecular-Dynamics (NEMD). Green-Kubo calculations are found to be very sensitive to the ill-defined partial enthalpy computation, resulting in an overestimation of the κ . However, the Green-Kubo and the direct method viscosity calculations demonstrate a reasonable agreement.

Following the more reliable method, the NEMD direct approach, κ of the nanofluids consisting of spherical nanoparticles with different diameters are investigated. The computational results are compared with the classical effective medium theories and no anomalous κ enhancements are observed in the nanofluids having fully dispersed spherical particles. Various microscopic mechanisms such as liquid layering and micro-convection are found to be ineffective for κ enhancements in nanofluids. However, greatly enhanced κ are achieved, a maximum of 63% relative to pure argon, in nanofluids consisting of chain-like particle arrangements. This demonstrates the potential origin of anomalous κ enhancements in experimental measurements and the capability of nanofluids with extended nanostructures to deliver better κ enhancements.

Further investigating the capability of extended nanostructures in nanofluid thermal transport, κ enhancements of nanofluids consisting of nanowires with different lengths and diameters are evaluated. It is shown that the heat conduction in the parallelly arranged liquid and the nanowires exhibit a coupled thermal behavior owing to the interface thermal resistance (R_b). This contradicts with the predictions of the classical

parallel heat conduction model and therefore, a novel model is proposed taking this coupled behavior into account. New heat transfer characteristics at the nanoscale are identified including the R_b -driven coupled heat conduction, the reduced κ of suspended nanowires, and the solid-like liquid layering. Using the new model, the importance of these microscopic thermal characteristics in accurately predicting the effective κ is shown. The sole contribution from the solid-like liquid layer to the κ enhancement is found to be in between 20-30% for the nanofluids considered.

Extending the investigation of heat transfer phenomena in nanofluids based on spherical nanoparticles, η of nanofluids with different nanoparticle sizes, concentrations, and arrangements are evaluated. Both the Green-Kubo and the direct methods are employed and unlike the κ , both methods show a reasonable agreement with one another. Viscosity is observed to decrease as the particle diameter increases in fully dispersed nanofluids. The ratio C_η/C_κ shows a decreasing trend indicating better heat transfer performance in nanofluids with large particles. Nanofluid η is observed to increase rapidly as the concentration increase. This makes C_η/C_κ to increase as well indicating the diminished heat transfer performance in nanofluids with high particle concentrations. As the particles in the nanofluid arrange into chain-like structures, η remains unaffected. This makes C_η/C_κ to decrease rapidly indicating the greater heat transfer performance in nanofluids with chain-like nanoparticle arrangements or in general, extended nanostructures.

Keywords: *Nanofluids, Nanoparticles, Nanowires, Thermal conductivity, Viscosity, Molecular dynamics*

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A	Cros-sectional area
Ar	Argon
C	Perimeter
Cu	Copper
C_η	Viscosity enhancement
C_κ	Thermal conductivity enhancement
D_n	Mass diffusion coefficient
D	Diameter
F	Force
f	Force or volumetric fraction
G	Heat flux
h	Enthalpy or partial enthalpy
h_b	Interface thermal conductance
J	Heat flux
k_B	Boltzmann constant
L	Length
m	Mass
N	Number of atoms
NPT	Isothermal-isobaric ensemble
NVE	Microcanonical ensemble
P	Stress tensor
p	Momentum
Q	Rate of heat transfer
R_b	Interface thermal resistance
R_{SV}	Interface surface area to volume ratio
r	Position vector or radius
T	Temperature
t	Time
U	Potential energy

V Volume

Greek symbols

ε Energy (kinetic and potential) / LJ energy scale

κ Thermal conductivity

η Viscosity

v Atomic velocity

σ LJ length scale

ω Phonon frequency

Subscripts

c Cross transfer

eff Effective

f,l Liquid

i,j Atomic index

m Continuous medium

s Solid

T Total

w Nanowire

Abbreviations

EM Effective medium

GK Green-Kubo

HCAF Heat current autocorrelation function

LAMMPS Large-scale atomic/molecular massively parallel simulator

LJ Lennard-Jones

MD Molecular dynamics

MEMS Micro-Electrical-Mechanical-System

MSD Mean square displacement

NEMD Non-equilibrium molecular dynamics

PHCM Simple parallel heat conduction model

RDF Radial distribution function

SLL	Solid-like liquid layer
VACF	Velocity autocorrelation function
VDOS	Vibrational density of states

Special notations

κ_S^{Bulk}	Bulk thermal conductivity of solid phase
$Eq. 4.31 _{\kappa_S^{Bulk}}$	Predictions via <i>Eq. 4.31</i> using bulk thermal conductivity of the solid phase
κ_w	Thermal conductivity of freestanding nanowires
κ_w^{Sus}	Thermal conductivity of nanowires suspended in a liquid
$Eq. 4.31 _{\kappa_w^{Sus}}$	Predictions via <i>Eq. 4.31</i> using the suspended nanowire thermal conductivity
κ_{SLL}	Thermal conductivity of the solid-like structured liquid
κ_{OL}	Thermal conductivity of the ordinary liquid
$Eq. 4.31 ^{SLL}$	<i>Eq. 4.31</i> including the effects of solid-like liquid layer
$Eq. 4.31 _{\kappa_w^{Sus}}^{SLL}$	Predictions via $Eq. 4.31 ^{SLL}$ using the suspended nanowire thermal conductivity
$Eq. 4.31 _{\kappa_S^{Bulk}}^{SLL}$	Predictions via $Eq. 4.31 ^{SLL}$ using the bulk thermal conductivity of the solid phase