A MOLECULAR DYNAMICS STUDY ON VISCOUS AND THERMAL PROPERTIES OF NANOFLUIDS

Chamara Nipun Somarathna

(208009D)

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Department of Mechanical Engineering

University of Moratuwa

Sri Lanka

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Declaration

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Mr. C.N. Somarathna — Date

The above candidate has carried out research for the master's dissertation under my supervision.

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Dr. Nalaka Samaraweera — Date

UOM Verified Signature

13/03/2023

Dr. Saliya Jayasekara — Date

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Prof. Kaþila Pērera — Date

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

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Abstract

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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Nomenclature

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
ν	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 *Eq. 4.31* 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 *Eq. 4.31* using the suspended nanowire thermal conductivity
κ_{SLL}	Thermal conductivity of the solid-like structured liquid
κ_{OL}	Thermal conductivity of the ordinary liquid
$Eq.\,4.31|^{SLL}$	*Eq. 4.31* including the effects of solid-like liquid layer
$Eq.\,4.31|^{SLL}_{\kappa_w^{Sus}}$	Predictions via $Eq.\,4.31|^{SLL}$ using the suspended nanowire thermal conductivity
$Eq.\,4.31|^{SLL}_{\kappa_s^{Bulk}}$	Predictions via $Eq.\,4.31|^{SLL}$ using the bulk thermal conductivity of the solid phase