EFFECT OF VOLUME FRACTION FOR DIFFERENT THERMOPHYSICAL PROPERTIES OF CARBON NANOTUBE NANOFLUID

NURADLIN ATHIRAH BINTI YAACOB

SCHOOL OF MECHANICAL ENGINEERING
UNIVERSITI SAINS MALAYSIA
2021

EFFECT OF VOLUME FRACTION FOR DIFFERENT THERMOPHYSICAL PROPERTIES OF CARBON NANOTUBE NANOFLUID

By :

NURADLIN ATHIRAH BINTI YAACOB

(Matrix Number : 137858)

Supervisor :

PROF.IR.DR.MOHD ZULKIFLY ABDULLAH

This dissertation is submitted to

UNIVERSITI SAINS MALAYSIA

As partial fulfilment of requirement for the degree of

BACHELOR OF ENGINEERING (HONS.) MECHANICAL ENGINEERING

School of Mechanical Engineering
Universiti Sains Malaysia
7 July 2021

DECLARATION

This work has not previously been accepted in substance for any degree and is not being concurrently submitted in candidature for any degree.

Signed:  (Nuradlin Athirah Binti Yaacob)

Date : 7th July 2021

STATEMENT 1

This thesis is the result of my own investigations , except where otherwise stated. Other sources are acknowledged by giving explicit references. Bibliography/references are appended.

Signed:  (Nuradlin Athirah Binti Yaacob)

Date : 7th July 2021

STATEMENT 2

I hereby give my consent for my thesis, if accepted, to be available for photocopying and for interlibrary loan, and for the title and summary to be made available outside organizations.

Signed:  (Nuradlin Athirah Binti Yaacob)

Date : 7th July 2021

ACKNOWLEDGEMENT

First & Foremost, I would like to express my biggest gratitude to God Almighty, Allah swt, with His Grace and Blessings, I was able to complete my Final Year project.

Next, a special thanks to my Final Year Project supervisor, Prof. Ir. Dr. Mohd Zulkifly Abdullah for his tremendous guidance and teachings throughout my journey of completing my Final Year project (FYP). With his great supervision and advices, I managed to finish my Final Year Project and thesis on time. His splendid and patience in teachings had improved my understanding on the overall topic of my Final Year Project, specifically on Molecular Dynamic (MD) Simulation by employing Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) with computation of Green Kubo method and the understanding on thermophysical properties of CNT nanofluids.

Next, I would also like to express my sincere thanks to my Final Year Project coordinator, Dr Muhammad Fauzinizam Bin Razali who had organized multiple online classes and seminars to help me get deeper understanding on how to write each section in thesis writing. Moreover, he had also given the thesis template/format as a guidance for us to write FYP thesis with a good format. Next, I would like to express my gratitude to School of Mechanical Engineering for giving me the opportunity to conduct this study with supervision under Prof. Ir. Dr. Mohd Zulkifly Abdullah.

Lastly, I would like to give a special thanks to my parents who had given me endless support in completing my Final Year Project (FYP). They had given moral support and splendid encouragement during the completion of my Final Year Project and Thesis writing.

ABSTRAK

Nanofluid terdiri daripada cecair asas dan naopartikel. Nanopartikel terdiri daripada 4 elemen iaitu logam, oksida, karbon dan juga nano-titisan. Terdapat pelbagai jenis nanopartikel karbon seperti Karbon Nanotube (CNT) dan Graphene. Pada masa kini, jenis yang paling biasa digunakan di kebanyakan industri ialah Karbon Nanotube kerana sifat termofisiknya yang hebat dan dapat membantu dalam aplikasi tertentu seperti aplikasi pemindahan haba, aplikasi bioperubatan (penyampaian nanodrug & terapi barah) dan penyejukan cip mikro. Terdapat dua cara untuk menentukan sifat termofizik iaitu dengan kaedah eksperimen dan simulasi. Walau bagaimanapun, kos untuk mengendalikan eksperimen adalah sangat mahal dan mengambil masa yang lama. Oleh itu, dalam kajian ini, Molekul Dinamik (MD) Simulasi dengan fomulasi Kubo Hijau telah diaplikasikan untuk mensimulasikan sifat termofisik Karbon Nanotube (CNT) nanofluid, khususnya kekonduksian terma, kelikatan dinamik, jumlah tenaga dan ketumpatan pada pecahan isipadu 2.7%, 2.9% dan 5.3% nanopartikel CNT . Hasil jumlah tenaga simulasi digunakan untuk mengira haba tertentu untuk Karbon Nanotube (CNT) nanofluid pada semua pecahan isipadu. Tujuan utamanya adalah untuk menentukan kesan pecahan isipadu terhadap sifat termofisik Karbon Nanotube (CNT) nanofluid. Kelikatan dinamik untuk Karbon Nanotube (CNT) nanofluid menunjukkan kenaikan sebanyak 0.5% hingga 0.6% manakala ketumpatan Karbon Nanotube (CNT) nanofluid menunjukkan kenaikan sebanyak 0.1% hingga 0.4% apabila pecahan isipadu meningkat. . Hasil haba tentu Karbon Nanotube (CNT) nanofluid menunjukkan pengurangan sebanyak 5% apabila pecahan isipadu meningkat. Hasil ini selaras dengan karya-karya penyelidikan yang telah dijalankan sebelum ini. Seterusnya, kekonduksian terma CNT nanofluid berkurang apabila pecahanan isipadu meningkat. Hasil kekonduksian terma CNT nanofluid ini adalah tidak tepat. Oleh itu, kekonduksian termal nanofluid CNT juga dikira dengan menggunakan Persamaan Maxwell dan hasilnya menunjukkan kenaikan sebanyak 1% hingga 6% apabila pecahan isipadu meningkat. Hasil ini selaras dengan karya-karya penyelidikan yang telah dijalankan sebelum ini.

ABSTRACT

Nanofluids comprise of base fluid and naoparticles. Nanoparticle comprises of 4 elements which are metallic, oxide, carbon and also nano-droplet. There are various types of carbon nanoparticle such as Carbon Nanotubes (CNTs) and Graphene. Nowadays, the most common types used in most industries is Carbon Nanotubes due to its great thermophysical properties which able to help in certain applications such as heat transfer application, biomedical application (nanodrug delivery & cancer therapeutics) and cooling of microchips. There are two ways in order to determine the thermophysical properties of nanofluid which are by experimental and simulation work. However, the experimental work is expensive, time – consuming and requires great effort and sufficient knowledge on the experimental procedure. Therefore, in this present study, Molecular Dynamic (MD) Simulation with computation of Green Kubo formularization had been carried out to simulate the thermophysical properties of CNT nanofluids, specifically thermal conductivity, dynamic viscosity, total energy and density at volume fraction 2.7%, 2.9% and 5.3% of CNT nanoparticles. The result of simulated total energy of CNT nanofluid was utilized to calculate specific heat of CNT nanofluid at all volume fraction stated above. The main aim is to determine the effect of volume fraction on the thermophysical properties of CNT nanofluids. The dynamic viscosity results of CNT nanofluid shows 0.5% to 0.6% increment when the volume fraction increases. The density results of CNT nanofluid shows 0.1% to 0.4% increment when the volume fraction increases. The specific heat results of CNT nanofluids shows 5% reduction when the volume fraction increases. These results are consistent with recent published work. Next, the thermal conductivity of CNT nanofluid shows reduction when volume fraction increases which is inaccurate. Hence, the thermal conductivity of CNT nanofluid was also calculated by using theoretical formulae of Maxwell Equation and the results shows 1% to 6% increment when the volume fraction increases. This result is consistent with recent published work.

TABLE OF CONTENTS

ACKNOWLEDGEMENT ..... **IV**

ABSTRAK ..... **V**

ABSTRACT ..... **VI**

TABLE OF CONTENTS ..... **VII**

LIST OF TABLES ..... **X**

LIST OF FIGURES ..... **XII**

LIST OF ABBREVIATIONS ..... **XIV**

CHAPTER 1 INTRODUCTION **1**

1.1 Overview 1

1.2 Problem statement 2

1.3 Objectives 3

1.4 Scope of project 3

CHAPTER 2 LITERATURE REVIEW **4**

2.1 Overview 4

2.2 Effect of volume fraction on thermophysical properties of nanofluids 5

2.2.1 Effect of volume fraction and temperature on dynamic viscosity of nanofluids 5

2.2.2 Effect of volume fraction on thermal conductivity nanofluids 11

2.2.3 Effect of volume fraction and temperature on density of nanofluids 13

2.2.4 Effect of volume fraction and temperature on specific heat of nanofluids 14

2.3 Interatomic potential definition 16

2.4 Molecular dynamic simulation 18

2.5 Summary of literature review 20

CHAPTER 3 METHODOLOGY **21**

3.1 Molecular dynamic simulation 23

3.2 Computation of thermophysical properties 31

3.2.1 Thermal conductivity 32

3.2.2 Specific heat 33

3.2.3 Dynamic viscosity 37

3.2.4 Density.....38

CHAPTER 4 RESULTS AND DISCUSSION.....39

4.1 Effect of volume fraction on thermal conductivity 39

4.2 Effect of volume fraction on specific heat 45

4.3 Effect of volume fraction on dynamic viscosity 49

4.4 Effect of volume fraction on density.....53

CHAPTER 5 CONCLUSION AND FUTURE RECOMMENDATIONS 57

5.1 Conclusion.....57

5.2 Recommendations for Future Research 59

REFERENCES.....60

APPENDIX A: LAMMPS INPUT CODE FOR THERMAL CONDUCTIVITY, DYNAMIC VISCOSITY, DENSITY AND TOTAL ENERGY OF BASE FLUID

APPENDIX B: 'SYSTEM.IN.INIT' & 'SYSTEM.IN.SETTINGS' CODE FOR BASE FLUID

APPENDIX C: LAMMPS CODE FOR DYNAMIC VISCOSITY, THERMAL CONDUCTIVITY, DENSITY AND TOTAL ENERGY OF CNT NANOFLUID (AT 2.7% VOLUME FRACTION)

APPENDIX D: 'SYSTEM.IN.INIT' AND 'SYSTEM.IN.SETTINGS' CODE OF CNT NANOFLUID (AT 2.7% VOLUME FRACTION)

APPENDIX E: LAMMPS CODE FOR DYNAMIC VISCOSITY, THERMAL CONDUCTIVITY, DENSITY AND TOTAL ENERGY OF CNT NANOFLUID (AT 2.9% VOLUME FRACTION)

APPENDIX F: 'SYSTEM.IN.INIT' AND 'SYSTEM.IN.SETTINGS' CODE OF CNT NANOFLUID (AT 2.9% VOLUME FRACTION)

APPENDIX G: LAMMPS CODE FOR DYNAMIC VISCOSITY, THERMAL CONDUCTIVITY, DENSITY AND TOTAL ENERGY OF CNT NANOFLUID (AT 5.3% VOLUME FRACTION)

APPENDIX H: ‘SYSTEM.IN.INIT’ AND ‘SYSTEM.IN.SETTINGS’ CODE OF CNT NANOFLUID (AT 5.3% VOLUME FRACTION)

LIST OF TABLES

Page

Table 2.1 Thermal conductivity of nanofluid for each volume fraction (Mohebbi, 2012) 12

Table 2.2 Density of SWCNT-water nanofluid for each volume fraction (Jabbari et al., 2017) 14

Table 3.1 Visualization of atoms in OVITO Software for each number of atoms . 25

Table 3.2 Radius of each atoms 27

Table 3.3 Volume fraction for each number of atoms 28

Table 3.4 Thermal Conductivity (using Maxwell Equation) of CNT nanofluid for each volume fraction 33

Table 3.5 Total Energy of base fluid at 308K and 313K 35

Table 3.6 Molar mass of Carbon Nanotube (CNT) and Water Molecule 35

Table 3.7 Total Energy of CNT nanofluid at 293K and 298K 36

Table 4.1 Table of Actual Thermal Conductivity, Simulated Thermal Conductivity and Total Energy of base fluid (water) at different temperature 39

Table 4.2 Simulated Thermal Conductivity (using Green Kubo) of CNT nanofluid for each volume fraction 41

Table 4.3 Results of Thermal conductivity of CNT nanofluid obtained by using Green Kubo method and Maxwell Equation for each volume fraction 43

Table 4.4 Actual Specific Heat of water, Results of Specific Heat of water from this work (using calculation) and Difference in Total Energy of base fluid (water) at different temperature 46

Table 4.5 Specific heat of CNT nanofluid for each volume fraction 47

Table 4.6 Results of actual dynamic viscosity and simulated dynamic viscosity for base fluid at each temperature 50

Table 4.7 Dynamic viscosity of CNT nanofluid for each volume fraction 51

Table 4.8 Actual Density and Calculated Density of base fluid (water) at a fixed temperature of 308K 53

Table 4.9 Actual Density and Simulated density of base fluid (water) for each temperature 54

Table 4.10 Density of CNT nanofluids for each volume fraction 55

LIST OF FIGURES

Figure 2.1 Experimetal results of dynamic viscosity of SWCNTs at various volume fraction and temperature of nanoparticles (Jabbari et al., 2019)..... 6

Figure 2.2 MD simulation results of dynamic viscosity of SWCNTs at various volume fraction and temperature of nanoparticles (Jabbari et al., 2019) 7

Figure 2.3 Viscosity MWCNTs at various volume concentration and temperature of MWCNTs (Premalatha & Jeevaraj, 2016)..... 8

Figure 2.4 Enhancement of shear viscosity of nanofluids versus volume fraction of nanoparticles (Jabbari et al., 2017) 9

Figure 2.5 Dynamic viscosity of CNT-water nanofluids at various temperature and volume fraction of nanoparticles (Jabbari et al., 2019) 10

Figure 2.6 Enhancement of thermal conductivity of nanofluids versus volume fraction of nanoparticles (Jabbari et al., 2017) 11

Figure 2.7 Thermal conductivity of nanofluids at various temperature and concentration of nanoparticles (Premalatha & Jeevaraj, 2016) 13

Figure 2.8 Specific heat of nanofluids at various temperature and volume fraction of Multi-Walled Carbon nanotube nanofluid (Thakur et al., 2017) 15

Figure 2.9 Specific heat of Indonesian fly ash nanofluids versus volume concentration of nanoparticles (Kanti et al., 2020)..... 16

Figure 3.1 Molecular Dynamic Simulation flowchart 23

Figure 3.2 Base fluid geometry..... 24

Figure 4.1 Graph of Actual Thermal Conductivity of base fluid versus Temperature of base fluid..... 40

Figure 4.2 Graph of Simulated thermal conductivity of water versus temperature of water..... 40

Figure 4.3 Graph of Simulated thermal conductivity (using Green Kubo) of CNT nanofluid versus volume fraction..... 42

Figure 4.4 Graph of thermal conductivity of CNT nanofluid (obtained using Maxwell Equation) versus volume fraction 44

Figure 4.5 Graph of Actual Specific heat of base fluid (water) versus Temperature of base fluid (water) 46

Figure 4.6 Graph of Calculated Specific heat of water versus temperature of water (base fluid) 47

Figure 4.7 Graph of Specific heat of CNT nanofluid versus volume fraction..... 48

Figure 4.8 Graph of Actual Dynamic Viscosity of base fluid versus Temperature of base fluid 50

Figure 4.9 Graph of Simulated Dynamic Viscosity of base fluid versus Temperature of base fluid..... 51

Figure 4.10 Graph of dynamic viscosity of CNT nanofluid versus volume fraction 52

Figure 4.11 Graph of Actual Density of base fluid versus Temperature of base fluid 54

Figure 4.12 Simulated Density of base fluid (water) versus Temperature of water55

Figure 4.13 Graph of density of CNT nanofluid versus volume fraction 56

LIST OF ABBREVIATIONS

CNT	Carbon Nanotube Nanofluid
MWCNT	Multi-Walled Carbon Nanotube
SWCNT	Single-Walled Carbon Nanotube
MD	Molecular Dynamic
VOL.	Volume
USM	Universiti Sains Malaysia
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
OVITO	Open Visualisation Tool

CHAPTER 1

INTRODUCTION

1.1 Overview

According to Jabbari et al.(2019), nanofluids was being introduced in the recent 1990s by an inventor named Choi who had the audacity and concept of inventing new type of fluids called nanofluids which is a nanometer-sized particles and made up of several materials such as metals, oxides, carbides and carbon nanotubes (Jabbari et al., 2019). Due to its good properties in terms of conductivity and viscosity as compared to conventional fluid, nanofluids able to be utilized in many applications including heat transfer application in several industries such as microelectronics industry, pharmaceutical industry and automotive industry (to improve hybrid-powered engines and vehicle thermal management) (Sadri et al.,2014). According to W Rashmi et al.(2014), there are actually various types of nanofluids which comprises of base fluid and nanoparticle (W Rashmi et al.,2014). Nanoparticle comprises of 4 elements which are metallic, oxide, carbon and also nano-droplet. There are various types of carbon nanoparticle such as Carbon Nanotubes (CNTs) and Graphene. Nowadays, the most common types used in most industries is Carbon Nanotubes (a type of nanoparticles) due to its great thermal and electrical conductivity, high viscosity and high tensile strength which able to help in certain applications such as heat transfer application, biomedical application (nanodrug delivery & cancer therapeutics) and cooling of microchips.

Generally, there were various researches conducted on thermophysical properties of nanofluids, specifically on thermal conductivity and viscosity using two methods which are experimental and simulation. However, the cost for conducting experimental investigation on nanofluids is very expensive and time-consuming. Therefore, certain researches carried out study on nanofluids by using simulation method. However, various problems and difficulties will be encountered if nanofluids is simulated by using other Computational Fluid Dynamics (CFD) Software because other CFD softwares unable to compute physical and chemical interactions of the system in nanofluid. Therefore, it is highly necessary to carry out nanofluid simulation using Molecular Dynamic (MD) Simulation. Plus, Molecular Dynamic (MD) Simulation consumes less cost, less time and produces results/output which is more accurate. Molecular dynamics (MD) is one of the effective simulation method which relates to Newton's equations of motion and is

computed for interacting and moving particles in order to observe trajectories of molecules, and their forces. According to Alkhwaji et al. (2020), there are two types of Molecular Dynamic (MD) Simulation which are Equilibrium molecular dynamics (EMD) and Non-equilibrium molecular dynamics (NEMD) methods (Alkhwaji et al., 2020). The EMD uses the Green-Kubo formula, in which computation and calculation is necessary and required, whereas in the NEMD method, a specific heat flux is restricted and the temperature gradient is determined.

The main aim of this project is to investigate the effect of volume fraction of Carbon Nanotube (CNT) nanofluid for different thermophysical properties, specifically on density, thermal conductivity, specific heat and dynamic viscosity by using Molecular Dynamic (MD) Simulation. Molecular Dynamic (MD) Simulation can be performed by employing LAMMPS software (Lee et al., 2016).

LAMMPS Software will be utilized to compute and simulate the Green Kubo formularization of Equilibrium Molecular Dynamic (EMD). Green-Kubo formularization of EMD method able to compute the thermal conductivity and dynamic viscosity using the fluctuation-dissipation theorem.

1.2 Problem statement

Nanofluids are extremely important due to its good mechanical properties which able to be utilized in areas involving heat transfer application and in automotive industry such as in hybrid powered engines. There are various types of nanofluids. However, in this project, Carbon Nanotube (CNT) Nanofluid is utilized due to its characteristic of high thermal & mechanical conductivity, low density and good in heat transfer application (Sivashanmugam, 2012). Carbon Nanotubes (CNT) nanofluid is utilized instead of water-base fluid because water-base fluid is not sufficient to cool down high heat flux during Molecular Dynamic Simulation.

Since experimental method of investigating nanofluids is expensive and time-consuming, thus simulations are widely utilized. Plus, although the results from experimental method is more genuine, however it requires great effort and sufficient knowledge on the experimental procedure. Due to this disadvantages and tremendous

advancement on computer and technology, many researches had carried out simulations on nanofluids which can only be conducted by using specific software such as Molecular Dynamic (MD) Simulations (Loya et al., 2014). Various problems and difficulties will be encountered if nanofluids is simulated by using other Computational Fluid Dynamics (CFD) Software because other CFD software unable to compute physical and chemical interactions of the system in nanofluid. Therefore, this project utilizes Molecular Dynamic (MD) Simulation by computing Green Kubo equations to conduct simulation on thermophysical properties of Carbon Nanotubes nanofluid (Loya, 2017).

1.3 Objectives

1. Able to investigate the effect of volume fraction of Carbon Nanotubes (CNT) nanofluid on different thermophysical properties such as thermal conductivity, dynamic viscosity, specific heat and density of Carbon Nanotubes (CNT) nanofluid.
2. Able to simulate and compute Green Kubo formularization of Equilibrium Molecular Dynamic Simulation by employing LAMMPS software to obtain value of thermal conductivity, dynamic viscosity, density and total energy of Carbon Nanotubes (CNTs) nanofluid at volume fraction 2.7%, 2.9% and 5.3%. The simulated total energy will be utilized to calculate the specific heat of Carbon Nanotubes (CNTs) nanofluid.

1.4 Scope of project

This present work conducted to study the effect of volume fraction on thermophysical properties, specifically on dynamic viscosity, thermal conductivity, specific heat and density of Carbon Nanotube nanofluid. The type of nanofluid used in this study is Carbon Nanotube (CNT) Nanofluid. The thermophysical properties of CNT nanofluid were investigated by using Molecular Dynamic (MD) simulation with Green Kubo method by employing LAMMPS. This limitation of this project is, unlike experimental work, it might not able to hold large atoms in the system due to the utilization of Molecular Dynamic simulation. The thermophysical properties of CNT nanofluids were investigated for three different volume fraction CNT nanofluid which are 2.7%, 2.9% and 5.3% in order to achieve the main objective of this study.

CHAPTER 2

LITERATURE REVIEW

2.1 Overview

Nanofluids was firstly introduced in the mid-1990 as colloidal suspensions which has an extremely small nanometer-sized particles which comprises of several particle such as metals, oxide, 62 carbide, nitrides and nanotubes dispersed in base fluid. Over the decades, nanofluids is the ultimate choice for certain application, specifically for heat transfer application due to its good characteritics in thermal conductivity and viscosity as compared to conventional fluids (Halelfadl et al., 2013). As discussed in Chapter 1, there were various applications involving nanofluids, including heat transfer application and automotive application in hybrid powered engines. Since mid-1990s, there were various researches who put great effort to extremely understand on the theories and mechanisms of nanofluids, specifically on the calculation of thermal conductivity using various methods. Therefore, there were various theoretical and simulation (empirical) studies which had been carried out in order to investigate the thermophysical properties of nanofluids (Jabbari et al., 2017). In simulation studies, most researches utilized Molecular dynamic (MD) simulation to determine and compute the thermophysical properties of nanofluids (Jabbari et al., 2017). The goal of this literature review is to compare the results of researches on thermophysical properties of nanofluids between experimental and simulation (empirical). The second goal of this literature review is to determine the gap between all the researches developed on thermophysical properties of nanofluids with this present work.

Volume fraction is one of the factors that will give impact to the characteristics, rheological and thermophysical properties (specifically thermal conductivity, viscosity, specific heat and density) of nanofluid. In this project, volume fraction can be defined as :

$$Volume\ fraction = \frac{volume\ fraction\ of\ nanoparticle}{volume\ fraction\ of\ nanofluid} \quad (2.1)$$

The increase in the volume fraction will result to higher volume of nanoparticles which are suspended in the base fluid. There are numerous researches that had been conducted on the effect of volume fraction in various thermophysical properties of nanofluids.

2.2 Effect of volume fraction on thermophysical properties of nanofluids

In this project, effect of volume fraction on thermophysical properties of Carbon Nanotubes (CNT) nanofluid are determined. This section will review the journals of experimental and simulation works related to thermopysical properties of nanofluids that had been carried out by various researches in order to be able to compare with the current results in this project.

2.2.1 Effect of volume fraction and temperature on dynamic viscosity of nanofluids

Dynamic viscosity is one of the most important flow characteristics of most fluids. Dynamic viscosity is the cause of resistance on the propagation between layers of fluids at various velocities. Dynamic viscosity is one of the important aspects to determine the thermophysical properties of nanofluids, specifically Carbon Nanotubes (CNTs) nanofluid. There are various researches conducted on the effect of volume fraction on dynamic viscosity of nanofluids using experimental and simulation method. In the aspect of effect of volume fraction on viscosity of nanofluids, Jabbari et al.(2019) carried out an experimental and simulation studies to measure and calculate the effects of volume fraction ranging 0.125%−1% and temperature ranging 25−65 °C on the dynamic viscosity of Single-Walled carbon nanotube (CNT) of water nanofluid. The experimental result shows that the dynamic viscosity of the nanofluid increases with increasing volume fraction of nanoparticles whereas dynamic viscosity of the nanofluid increases with decreasing temperature as shown in the graph of experimental of dynamic viscosity of SWCNTs at various volume fraction of nanoparticles as shown in below :

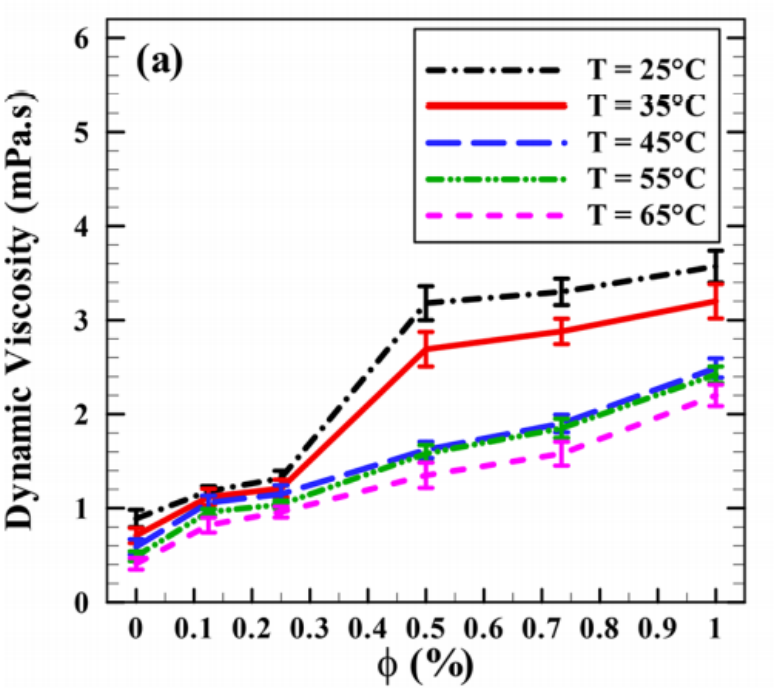

Figure 2.1 Experimetal results of dynamic viscosity of SWCNTs at various volume fraction and temperature of nanoparticles (Jabbari et al., 2019)

This is due to the higher forces attraction between nanoparticles and water which results to decrease in the momentum transfer between nanofluid layer. This will eventually lead to increase in dynamic viscosity of SWCNTS- water nanofluid. However, the simulation studies which was conducted by using Green Kubo formularization of Equilibrium Molecular Dynamic Simulation also produces the same results as in experimental method in which increasing volume fraction of nanoparticles will result to higher dynamic viscosity of the nanofluid whereas dynamic viscosity of the nanofluid increases with decreasing temperature as shown in the graph of MD simulation of dynamic viscosity of SWCNTs at various temperature and volume fraction of nanoparticles below :

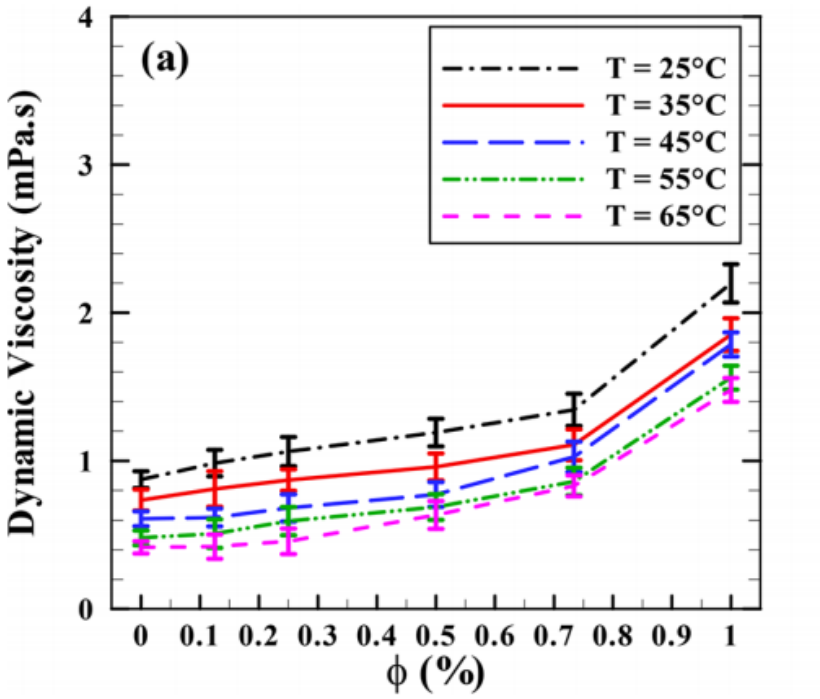

Figure 2.2 MD simulation results of dynamic viscosity of SWCNTs at various volume fraction and temperature of nanoparticles (Jabbari et al., 2019)

Premalatha & Jeevaraj, (2016) carried out an experiment on the effect of different temperatures (303 K, 308 K, 313 K, 318 K, and 323 K) and different volume concentration ranging (0–0.005 wt%) for viscosity of nanofluids. In this experiment, Multi-Walled Carbon Nanotube (MWCNTs)- Dowtherm A nanofluids is measured experimentally by utilizing Brookfield Company (USA) DV-II þ Pro Viscometer by rotational method. The result shows that increasing volume fraction of nanoparticles will undeniably increases the dynamic viscosity of MWCNTs nanofluid whereas decreasing temperature results to increasing dynamic viscosity of MWCNTs nanofluid (which satisfies the results from (Jabbari et al., 2019)). The diagram below shows graph of dynamic viscosity at various temperature and volume concentration of MWCNTs :

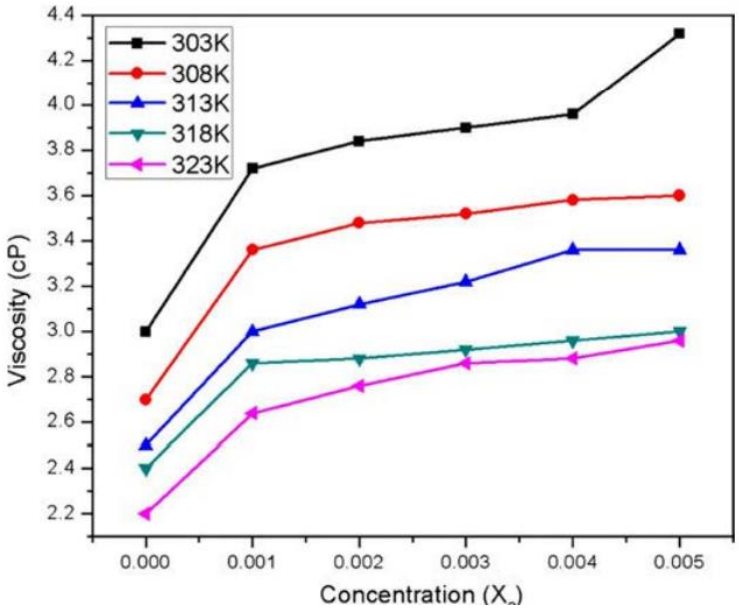

Figure 2.3 Viscosity MWCNTs at various volume concentration and temperature of MWCNTs (Premalatha & Jeevaraj, 2016)

According to Mehrali et al.(2014), higher volume concentration will result to agglomeration of nanoparticles in the solution. This will lead to higher shear stress of nanofluid due to the massive force required to eliminate the solid element of dispersion, therefore this will result to increase in the dynamic viscosity of MWCNTs.

Halelfadl et al. (2013) and Kanti et al.(2020) also carried out the experimental studies on the effect of different volume fractions and different temperatures on dynamic viscosity of carbon nanotubes (CNTs) water based nanofluids. These two researches also produced the same results as in the previous journals mentioned above in which increasing volume fraction of nanoparticles will undeniably increases the dynamic viscosity of nanofluids. According to Kanti et al.(2020), difference in size of particle and surfactant presence will significantly influenced the viscosity of nanofluids at different concentration.

In addition, there are also several simulation studies that had been carried out by Jabbari et al.(2017) and Cygan et al.(2004). Jabbari et al. (2017) conducted a molecular dynamic simulation on effects of volume fraction of nanoparticles for viscosity and thermal conductivity of nanofluids by using Green Kubo formularization of Equilibrium Molecular dynamic Simulation (EMD) with LAMMPS software. The simulation system was done by using water as base fluid in the simulatiom box with a quantity of 12 240 atoms simple cubic cell 50 Å in length, and by placing SWCNTs (with zigzag

geometry) at the centre. The initial arrangement of nanofluid system with 3d-computing domain was initially tempered in a NVE ensemble with the application of Langevin thermostat, then eventually the system operated in isothermal-isobaric ensemble (NPT). The result shows that increase in volume fraction of nanoparticles will undeniably increases the dynamic viscosity of nanofluids as shown in the graph of viscosity of nanofluids versus volume fraction of nanoparticles :

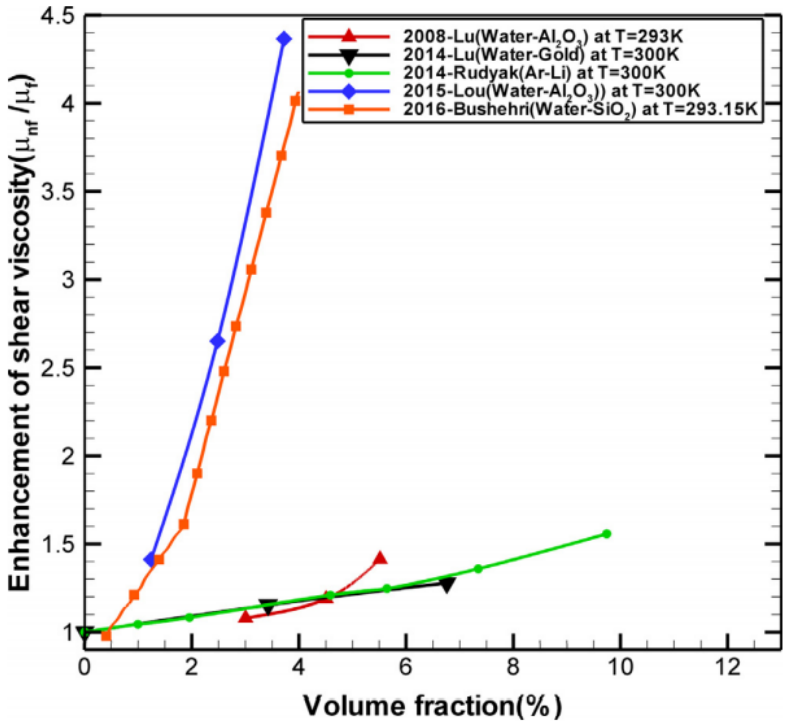

Figure 2.4 Enhancement of shear viscosity of nanofluids versus volume fraction of nanoparticles (Jabbari et al., 2017)

Cygan et al.(2004) also reported that higher volume fraction will result to higher dynamic viscosity of nanofluids. According to data of results reported by Cygan et al., (2004), when volume fraction of nanoparticle increased from 1.24% to 3.72%, the shear viscosity increased from 1.21 mPa s to 3.68 mPa s.

In the aspect of effect of temperature to viscosity of nanofluids, According to Jabbari et al.(2019) who also investigated the effect of temperature on dynamic viscosity of CNT-water nanofluid using Green Kubo formularization of Molecular Dynamic simulation method, the dynamic viscosity of CNT-water nanofluids decreases with an increase in temperature as shown in the graph of dynamic viscosity of CNT-water nanofluids at various temperature and volume fraction of nanoparticles below :

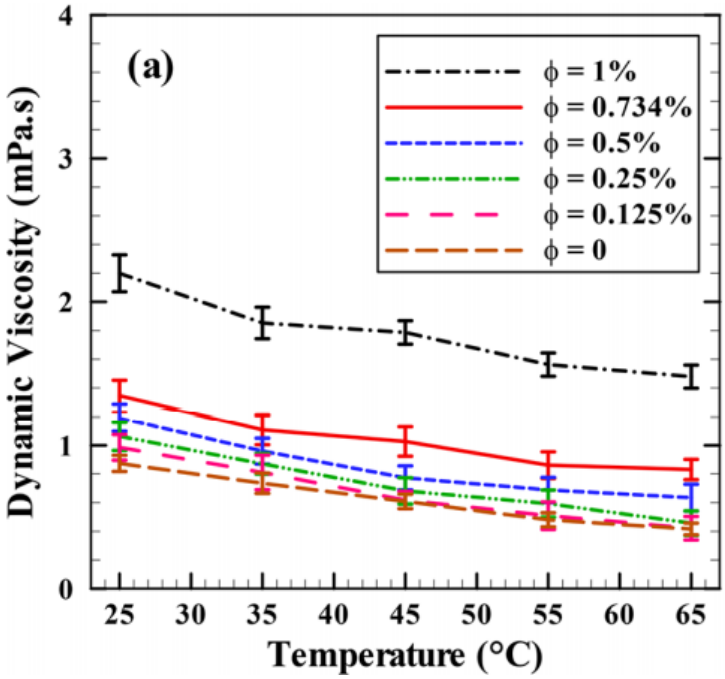

Figure 2.5 Dynamic viscosity of CNT-water nanofluids at various temperature and volume fraction of nanoparticles (Jabbari et al., 2019)

This is due to the easily removal between CNTs and water atoms due to higher kinetic energy caused by higher temperature which will lead to reduce in viscosity. Moreover, Thakur et al.(2017) and Vakili-Nezhaad & Dorany,(2012) also carried out the experimental studies to investigate the effect of different temperatures on viscosity of nanofluids. These researches also states that temperature is inversely proportional to viscosity of nanofluids in which when the temperature increases, the viscosity of nanofluids will decrease.

Lou & Yang,(2015) also reported that an increasing temperature will result to decreasing viscosity. This is because,at high temperature, the constraints between nanoparticles and base fluid are easily removed, and for this reason, the viscosity decreases at high temperature (Jabbari et al., 2017).

According to the results above, it is clearly observed that the results of effect of volume fraction and temperature on viscosity of nanofluids are accurately the same for both methods (experimental and simulation) in which dynamic viscosity of nanofluid increases with an increase in volume fraction whereas dynamic viscosity decreases with increasing nanofluid temperature.

2.2.2 Effect of volume fraction on thermal conductivity nanofluids

Thermal conductivity of a material defines the ability of the specific material to conduct heat. Thermal conductivity is one of the utmost important thermophysical characteristics in determining the heat transfer performance of nanofluids. In terms of effect of volume fraction for thermal conductivity using simulation method, Jabbari et al.(2017) who also investigated the effect of volume fraction on thermal conductivity of CNT-water nanofluid using Green Kubo formularization of Molecular Dynamic simulation method states that increase in volume fraction of nanoparticles will increase the thermal conductivity of CNT-water nanofluids as shown in the graph of enhancement of thermal conductivity of nanofluids versus volume fraction of nanoparticles below :

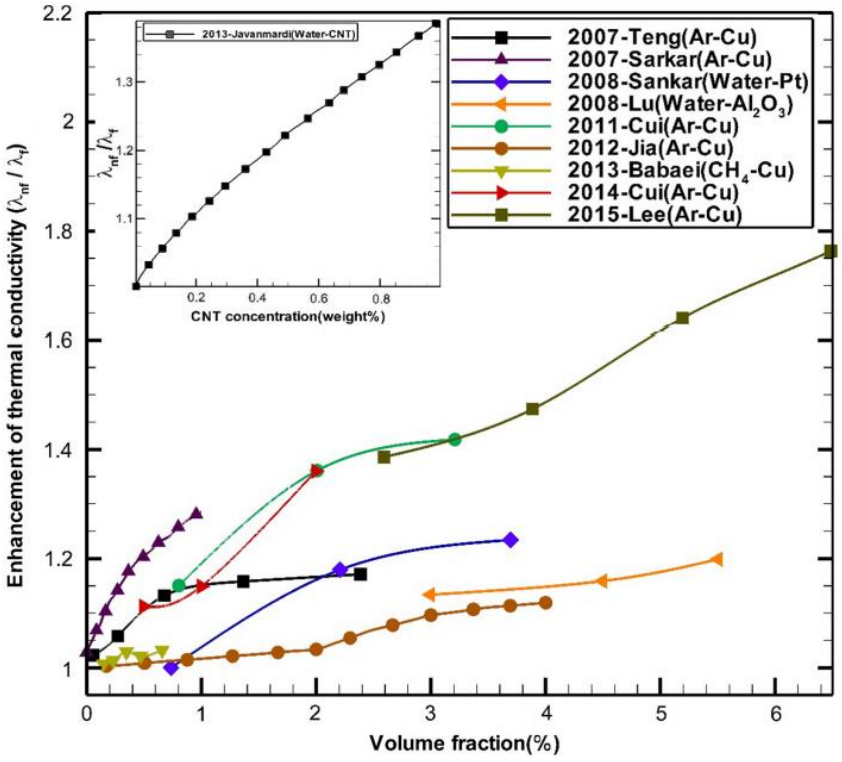

Figure 2.6 Enhancement of thermal conductivity of nanofluids versus volume fraction of nanoparticles (Jabbari et al., 2017)

On the other hand, Mohebbi, (2012) conducted simulation studies by combining equilibrium and non-equilibrium molecular dynamic simulation to compute thermal conductivity of nanofluid of silicon nitride nanoparticles in a liquid argon. CHARMM22 force field and NVT ensemble (in which total

number of atoms, system volume and temperature were all remain the same throughout the simulation) was also utilized to implement the simulation. The results shows that increase volume fraction of nanoparticles will increase the thermal conductivity of nanofluids in which the thermal conductivity value of 0.08 W/m K and 0.085 W/m K for 1.77% and 3.1% nanofluids, respectively as shown below :

Table 2.1 Thermal conductivity of nanofluid for each volume fraction (Mohebbi, 2012)

Thermal conductivity (W/mK)	Volume Fraction (%)
0.08 W/m K	1.77%
0.085 W/m K	3.1%

According to data provided by Sarkar and Selvam (2007), the thermal conductivities were 0.156 W/m K and 0.165 W/m K for 1% and 2% nanofluids, respectively in which the thermal conductivities increases with increasing volume fraction of nanofluids. In addition, Premalatha & Jeevaraj (2016) also carried out an experiment on the effect of volume concentration on thermal conductivity of MWCNT–Dowtherm A nanofluids using a transient heated needle (KD2 Pro, Decagon Devices, Inc., Pullman, WA, USA) which was able to calculate and measure experimentally the thermal conductivity of nanofluids with 5% accuracy. The results shows that higher volume concentration/volume fraction will result to higher thermal conductivity of nanofluids.

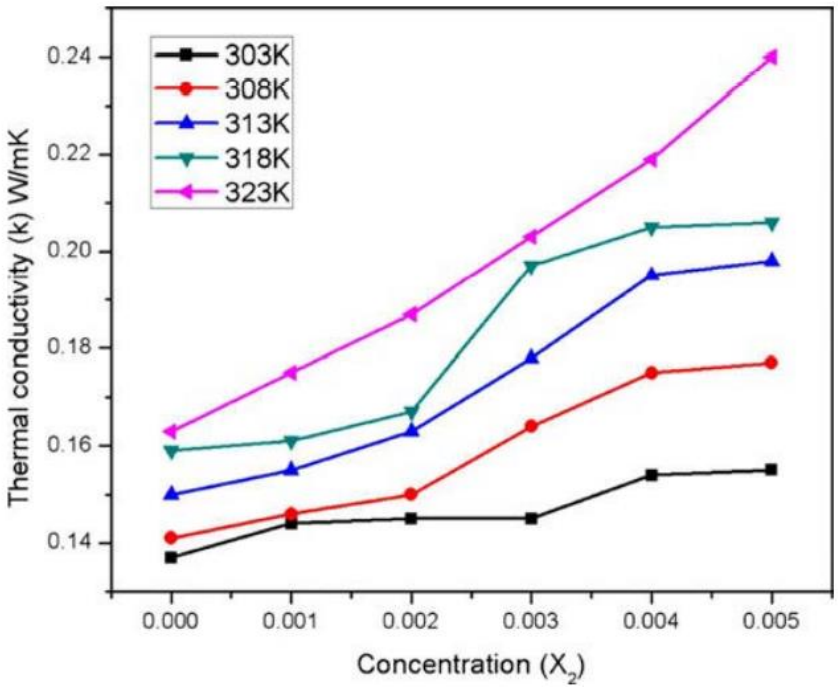

Figure 2.7 Thermal conductivity of nanofluids at various temperature and concentration of nanoparticles (Premalatha & Jeevaraj, 2016)

According to the results above, it is clearly observed that the results of effect of volume fraction on thermal conductivity of nanofluids are accurately the same for both methods (experimental and simulation) in which higher volume fraction will result to higher thermal conductivity of nanofluids.

2.2.3 Effect of volume fraction and temperature on density of nanofluids

In terms of effect of temperature and volume fraction on density of nanofluids using simulation method, Jabbari et al. (2017) states that higher volume fraction will result to higher density and higher temperature will result to lower the density. According to the data provided by Jabbari et al. (2017), the densities of SWCNT−water nanofluids were calculated as 1014.71, 1017.65, 1019.95, 1022.74, and 1025.43 kg/m3 with nanoparticle concentrations of 0.125, 0.25, 0.5, 0.734, and 1%, respectively.

Table 2.2 Density of SWCNT-water nanofluid for each volume fraction (Jabbari et al., 2017)

Volume fraction (%)	Density (g/cm^3) of SWCNT-water nanofluid
0.125	1.0147
0.25	1.0177
0.5	1.01995
0.734	1.023
1	1.025

2.2.4 Effect of volume fraction and temperature on specific heat of nanofluids

Specific Heat of a material can be defined as the volume of capacity of heat (rate of heat absorption and heat release) of a material per mass of the material. Specific heat is the utmost significant in determining the thermophysical properties of nanofluids. This is because if the specific heat of nanofluids is at a higher rate, massive amount of heat is allowed to be absorbed without requiring to increase the temperature. Thakur et al., (2017) recently conducted experimental studies in which the main aim is to investigate the effect of different volume fraction ranging 0 – 0.8 vol. % and different temperature ranging 30°C to 70°C on thermophysical properties of nanofluids such as thermal conductivity, specific heat, density and viscosity. The specific heat of MWCNT nanofluid was experimentally measured by utilizing DSC 4000 model (Differential Scanning Calorimeter, Perkin Elmer, USA). According to the graph below, the specific heat of nanofluid was measured at different concentrations/volume fraction (0%, 0.2%, 0.4%, 0.6% and 0.8%) and different temperatures (30°C, 40°C, 50°C, 60°C, 70°C). The result shows that the specific heat of MWCNT nanofluid increases with an increase in temperature. However, higher volume concentration/volume fraction of nanoparticles will result to lower specific heat of MWCNT nanofluid as shown in the graph below :

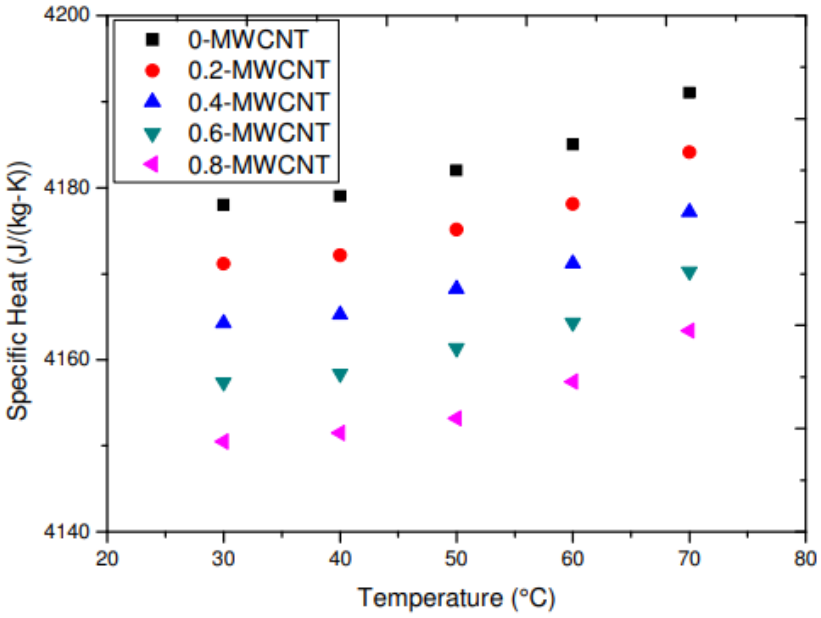

Figure 2.8 Specific heat of nanofluids at various temperature and volume fraction of Multi-Walled Carbon nanotube nanofluid (Thakur et al., 2017)

On the other hand, Kanti et al., (2020) conducted an experimental research on the effect of volume concentration/volume fraction of nanoparticles on Indonesian fly ash nanofluid with different volume concentration/volume fraction ranging 0.1–0.5% with different temperature ranging 30^0C–60^0C. by utilizing Differential Scanning Calorimeter (Model: DSC 7020, SII instruments, Japan) with 5% accuracy. The results shows that higher volume concentration/volume fraction of nanoparticles will result to lower specific heat as shown in the graph of specific heat versus volume concentration/volume fraction below :

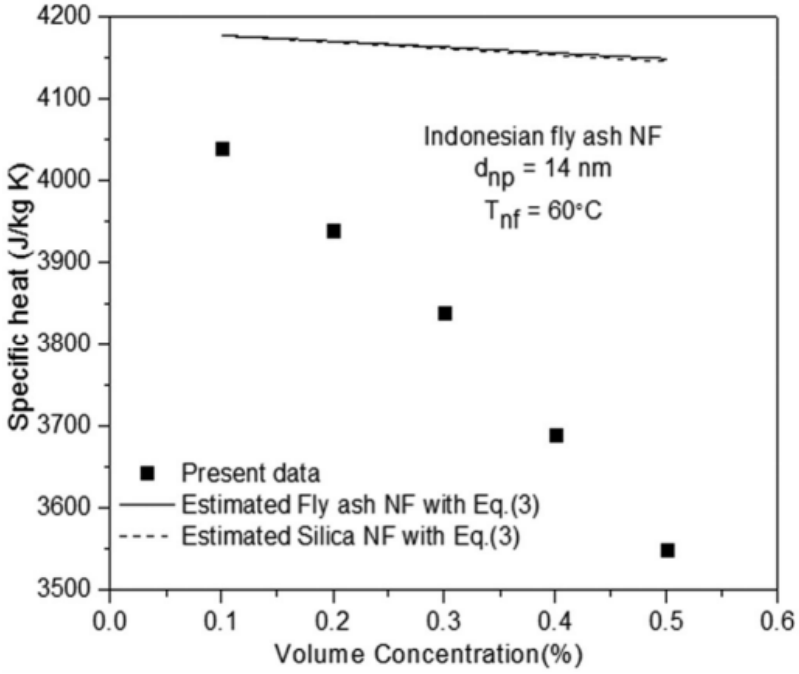

Figure 2.9 Specific heat of Indonesian fly ash nanofluids versus volume concentration of nanoparticles (Kanti et al., 2020)

This is because the specific heat of nanoparticles is lower as compared to that of base fluid. It can be implied that decrease in heat input is needed to high up the temperature of nanofluid at greater particle volume concentration. Therefore, lower specific heat will result to increase in nanofluid's convective heat transfer.

2.3 Interatomic potential definition

Interatomic potential is related to attractive or repulsive behaviour. There is a specific state which called atomistic equilibrium state. In interatomic interaction, there is a relation between atomic distance and repulsive force in which atomic distance is indirectly proportional to repulsive force. Shorter atomic distance will result to higher repulsive force (Chwał & Muc, 2020). Interatomic potential is extremely essential in Molecular Dynamic Simulation due to the dependency of the interactions between atoms on the interatomic defined potentials. This current work includes two types of interatomic potentials which are Morse, Tersoff-Brenner potentials for Carbon nanotube and Lennard-Jones potential for both base fluid and Carbon Nanotube (CNT)

(Senior, 1924). First and foremost, below shows the formularization of Lennard-Jones potential :

$$U(r_{ij}) = 4 \in \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]; (r_{ij} < r_{cutoff} \quad (2.2)$$

In which r_{ij} is referring to the distance between atom i and atom j whereas $\in$ and σ are the variables of Lennard-Jones potential. This current work utilizes Lennard-Jones potential together with long-range Coulumb in order for the interaction of water molecules in which between H-H bond (between hydrogen and hydrogen atoms) and between O-O bonds (between oxygen and oxygen atoms). Nevertheless, Lorentz Berthelot (LB) mixing rule the interaction between different atoms which is between H-O bond (between hydrogen and oxygen atom). below shows the formularization of Lorentz Berthelot (LB) mixing rule (M.P.Allen et.al, 1987):

$$\in_{ij} = \sqrt{\in_i \in_j} \quad (2.3)$$

$$\sigma_{ij} = \frac{1}{2}\sigma_i + \sigma_{ij} \quad (2.4)$$

Secondly, the interatomic potential which can be used for Carbon Nanotube are Morse and Tersoff-Brenner potentials which is described as below (Chwał & Muc, 2020) :

Morse potential can be defined as (Chwał & Muc, 2020) :

$$V^M(r_{ij}) = {D_e}^M[e^{-2\beta^{M(r_{ij}-R_{ij})}} - 2e^{-\beta^{M(r_{ij}-R_{ij})}}, \quad (2.5)$$

In which ${D_e}^M$ is referring to potential minimum whereas β^M is a constant corresponding to the atoms level. The interatomic force of Morse potential can be defined as (Chwał & Muc, 2020) :

$$F^M = 2\beta^M {D_e}^M \left[e^{-2\beta^{M(r_{ij}-R_{ij})}} - 2e^{-\beta^{M(r_{ij}-R_{ij})}}\right] \quad (2.6)$$

Next, Tersoff-Brenner potential which can be utilized for carbon atoms can be defined as (Chwał & Muc, 2020) :

$$V^{TB}(r_{ij}) = {V_R}^{TB}(r_{ij}) - \bar{B}_{ij}{V_A}^{TB} r_{ij} \quad (2.7)$$

$${V_R}^{TB}(r_{ij}) = f^{TB}(r_{ij}) \frac{{D_e}^{TB}}{S^{TB} - 1} e^{-\sqrt{2S^{TB}}\beta^{TB}(r_{ij} - R_{ij})} \quad (2.8)$$

$${V_A}^{TB}(r_{ij}) = f^{TB}(r_{ij}) \frac{{D_e}^{TB} S^{TB}}{S^{TB} - 1} e^{-\sqrt{\frac{2}{S^{TB}}}\beta^{TB}(r_{ij} - R_{ij})} \quad (2.9)$$

In which ${V_R}^{TB}$ and ${V_A}^{TB}$ are referring to repulsive and attractive parts, respectively. $f^{TB}(r_{ij})$ is the cut off function whereas $\bar{B}_{ij}$ is the "order" of atomic bonds. The interatomic force of Tersoff-Brenner potential can be defined as (Chwał & Muc, 2020) :

$$F^{TB} = \frac{\beta^{TB} {D_e}^{TB}}{S^{TB} - 1} [\sqrt{2S^{TB}} e^{-\sqrt{2S^{TB}}\beta^{TB}(r_{ij} - R_{ij})} - \bar{B} S^{TB} \sqrt{\frac{2}{S^{TB}}} e^{-\sqrt{\frac{2}{S^{TB}}}\beta^{TB}(r_{ij - R_{ij}})} \quad (2.10)$$

Next, Lennard-Jones potential which can be utilized for carbon nanotubes can be defined as (Chwał & Muc, 2020) :

$$V^{LJ}(r_{ij}) = \frac{B^{LJ}}{{r_{ij}}^{12}} - \frac{A^{LJ}}{{r_{ij}}^{6}} \quad (2.11)$$

In which A^{LJ} and B^{LJ} are both Lennard-Jones potential constants. $V^{LJ}(r_{ij})$ is representing repulsive forces whereas the right hand-sided component (which are $\frac{B^{LJ}}{{r_{ij}}^{12}} - \frac{A^{LJ}}{{r_{ij}}^{6}}$) are representing attractive forces.

2.4 Molecular dynamic simulation

Molecular Dynamic is a type of computer simulation method which is utilized to study and investigate the trajectories and motion of atoms, specifically nanoparticles. Molecular Dynamic involves the macroscopic and microscopic level of information in which macroscopic information includes pressure, energy and heat capacity whereas microscopic information includes the position and velocity of atoms (R Development Core Team, 2011). While carrying out Molecular Dynamic Simulation, the atoms or molecules interact and bonded with each other in the simulation box for certain interval of time. Therefore, this shows that the system able to mimic the condition and

movement of atoms in the real world and thus allows us to analyse the dynamic evolution of the system.

The trajectories of the atoms in the system can be computed by using a specific numerical method which is Newton's equations of motion in which the forces between particles and potential energies are taken into consideration as shown below (Loya et al., 2014):

$$F_i x_i = -\nabla_i U(x)_i \tag{2.12}$$

In which

$F_i(x)_i$ = forces exerted between particles whereas U(x) is referring to the potential energy between particles.

However, the acceeration of the atoms can be calculated by using Newton's Second Law of Motion :

$$F_i = ma_i \tag{2.13}$$

In which m = mass of atoms whereas a = acceleration of atoms.

The velocity and position of atoms can be calculated by using a specific numerical formulae as shown below:

$$v_i = {v_i}^o + a_i t \tag{2.14}$$

$$r_i = {r_i}^o + v_i t + \frac{1}{2} a_i t^2 \tag{2.15}$$

In which v_i is referring to the velocity of atom i, t is referring to time and r_i is the position of atom i. The trajectories of atoms in the system able to be configured over certain interval of time. The thermophysical properties can be obtained depending on the trajectories of atoms in accordance to the statistical mechanics.

2.5 Summary of literature review

According to the literature review, there are numerous researches done their researches on the effect of volume fraction to the thermal conductivity, dynamic viscosity and density of nanofluids by using Molecular Dynamic Simulation method. There are various experimental study conducted on the effect of volume fraction to specific heat of nanofluid. However, there is none Molecular Dynamic simulation research study regarding the effect of volume fraction on the specific heat of nanofluids. Therefore, in order to bridge the gap, in this project, the effect of volume fraction is analysed for various different thermophysical properties, including density, specific heat, thermal conductivity and dynamic viscosity. According to the literature review, most researches utilized Green Kubo of Equilibrium Molecular Dynamic (EMD) Simulation for computing different thermophysical properties of nanofluids since the method is efficient. This project will also be utilizing Molecular Dynamic (MD) Simulation with computation of Green Kubo and employing LAMMPS Software.

According to the literature review, the results obtained from simulation and experimental are accurately the same in which :

- In terms of effect volume fraction on dynamic viscosity of nanofluids, increase in volume fraction of nanoparticles will undeniably increases the dynamic viscosity of nanofluids.
- In terms of effect of temperature for dynamic viscosity of nanofluids, dynamic viscosity decreases with increasing nanofluid temperature.
- In terms of effect of volume fraction for thermal conductivity, higher volume fraction of nanoparticles will result to higher thermal conductivity of nanofluids.
- In terms of effect of temperature and volume fraction for density of nanofluids, higher volume fraction of nanoparticles will result to higher density of nanofluids and higher temperature of nanofluids will result to lower the density of nanofluids at the same volume fraction.
- In terms of effect of volume fraction for specific heat of nanofluids, higher volume fraction of nanoparticles will result to lower specific heat of nanofluids and higher temperature will result to higher the specific heat at the same volume fraction.

CHAPTER 3

METHODOLOGY

Since 1990s, Green Kubo formularization had been widely utilized in obtaining base fluids' and nanofluids' thermophysical properties by most researches. The result of thermophysical properties of base fluid by using G-K method was validated by making a detailed comparison with the actual result. However, the comparison between the actual result and simulation result leads to huge percentage error. This is because the researches did not use NPT or NVT ensemble in their simulation system which leads to high inaccuracy of the results. The usage of thermodynamic ensembles (NPT/NVT ensemble) are extremely important due to its ability to resemble the experimental condition in laboratory. NPT ensemble represents contant pressure and constant temperature whereas NVT ensemble represents constant volume and constant temperature. In this study, NVT ensemble was used for simulation of characteristics of base fluid and the simulation of characteristics of Carbon Nanotube (CNT) nanofluid due to its ability to obtain higher accuracy of results as compared to NPT ensemble.

In this current work, the thermophysical properties of base fluids and nanofluids were studied and investigated. Each thermophysical properties has their own unique relation with another different properties. For instance, thermal conductivity is related to the transmission of kinetic and potential energy of molecules whereas dynamic viscosity is related and influenced by the stress tensor of particles. Plus, specific heat is influenced by the total energy. These relations were analysed in order to obtain highly accurate result of thermophysical properties of nanofluids.

In this current research, the procedure (methodology) is divided into two parts which are which are MD Simulation and data analysis in which MD Simulation was utilized to collect data and results of thermophysical properties, including thermal conductivity, dynamic viscosity, total energy and density of base fluid and nanofluids. Then, the data and results were filtered, analysed and plotted into graph using Microsoft Excel. First and foremost, the Molecular Dynamic simulation is carried out initially on base fluid. This is because the actual value of thermophysical properties of base fluid is fixed and known. The results on simulated density, total energy, thermal conductivity and dynamic viscosity of base fluid were obtained by using Green Kubo formularization for 4 different temperatures (308K, 313K, 333K and 343K). The simulated result of

total energy from simulation represents the sum of kinetic energy and potential energy. The simulated result of total energy was utilized to obtain the specific heat of base fluid by using formula below :

$$\Delta Q = mc_p \Delta T \quad (3.1)$$

In which :

ΔQ = Difference in Total energy (J)

m = mass (kg)

c_p = specific heat (J/kgK)

Then, the actual value and simulation results (for each thermophysical properties of base fluid) were compared to ensure reliable results obtained from MD simulation. After finishing the simulation of thermophysical properties of base fluid, the simulation of thermophysical properties of Carbon Nanotube nanofluids were carried out. The simulation of thermophysical properties, including density, thermal conductivity and dynamic viscosity of Carbon Nanotube nanofluid was conducted by using the same step as in base fluid for three different volume fractions of Carbon nanotube nanofluid (CNT) which are at 2.7%, 2.9% and 5.3% at a fixed temperature and pressure of 298K and 1 atm repectively. However, since the calculation of specific heat requires two different total energy at two different temperature in order to obtain difference in total energy, ΔQ and difference in temperature ΔT, therefore the simulation of total energy of CNT nanofluid was also conducted for three different volume fraction of CNT nanofluid (2.7%, 2.9% and 5.3%), but at two different temperatures which are 293K and 298K.

3.1 Molecular dynamic simulation

In this project, Molecular Dynamic (MD) Simulation was implemented by employing Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software to compute Green-Kubo (G-K) formularization. G-K formularization involves NVT/NPT ensemble which relates to heat flux autocorrelation function. In this present study, NVT ensemble is used for the simulation of thermophysical properties of base fluid and the simulation of thermophysical properties of Carbon Nanotube nanofluids. The flowchart of Molecular Dynamic Simulation is shown below (Loya et al., 2014) :

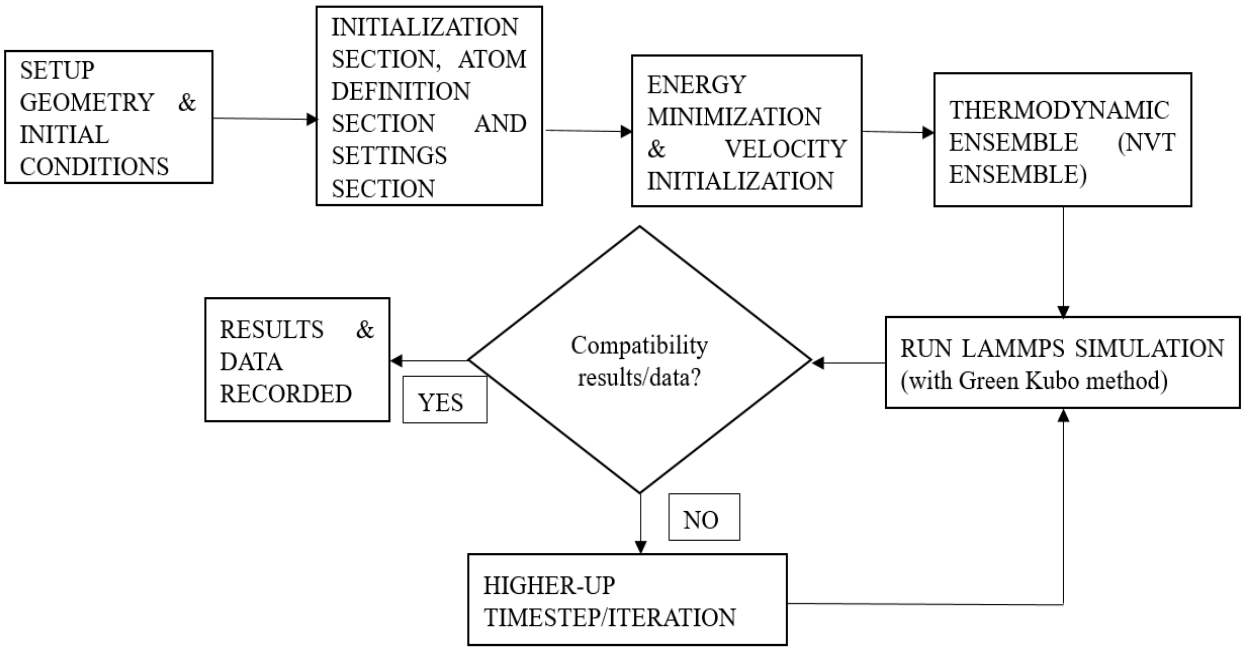

Figure 3.1 Molecular Dynamic Simulation flowchart

First and foremost, the system's geometry was generated. In this system, the geometry of water which acts as the base fluid was generated by utilizing Molecule builder software, also known as moltemplate. In this system, there are a total of 3000 atoms altogether. Since one molecule of water (H_2O) is comprising of 3 atoms which are 2 hydrogen atoms and 1 oxygen atom, thus:

$$= \frac{Number\ of\ water\ molecules}{Total\ Number\ of\ atoms\ in\ the\ system} \quad (3.2)$$
$$Total\ number\ of\ atoms\ in\ one\ molecule\ of\ water$$
$$= \frac{3000}{3} = 1000\ molecules\ of\ water$$

Therefore, in this system, there are 1000 molecules of water.

The water molecule was kept in a specific file in moltemplate, in which the file format able to imitate LAMMPS data file format containing specific 'Atoms' and 'Angles' sections. The water geometry system in moltemplate was set up as SPCE (Extended Simple Point Charge water model) which involves the specification of three-site rigid water molecule. There is a specific command ('fix rattle') utilized in moltemplate to properly fix interatomic bonds and angles of O-H to prevent breakage of the molecules. In this system, Periodic 19 boundary condition (PBC) was applied and utilized in order to ensure the resemblance of real life condition in the system simulation. Plus, PBC able to prevent the cross-over of bonds beyond the simulation box. The diagram below shows the visualization of base fluid geometry using OVITO Software:

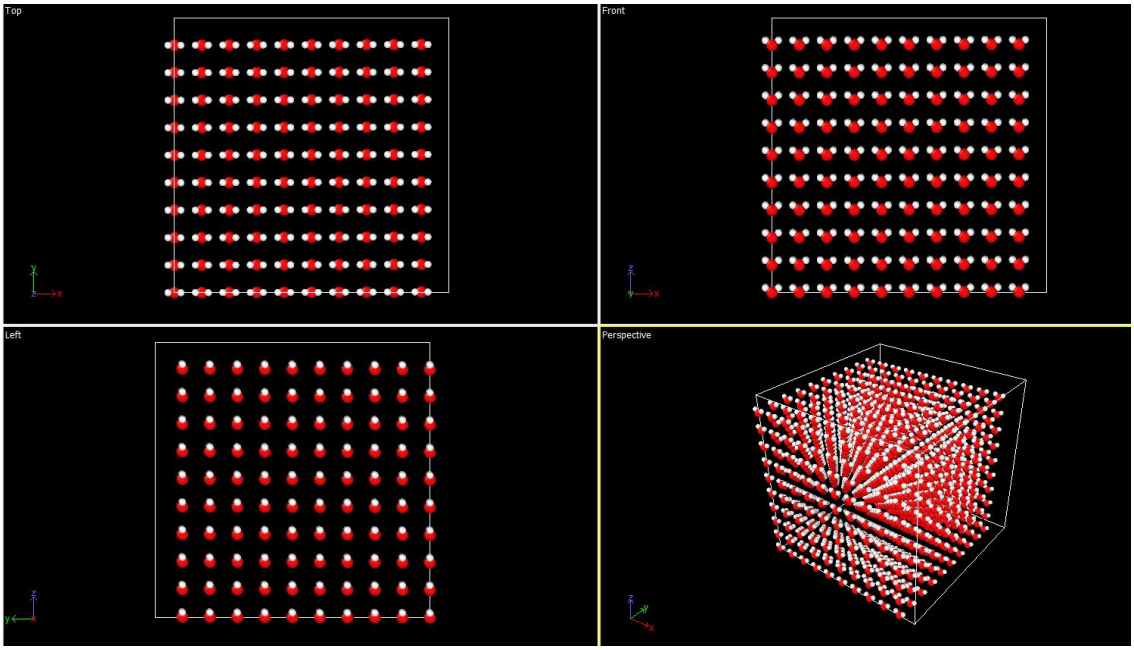

Figure 3.2 Base fluid geometry