FLUID FLOW THROUGH CARBON NANOTUBES AND GRAPHENE BASED NANOSTRUCTURES

A Thesis

Presented to
The Graduate Faculty of The University of Akron

In Partial Fulfillment
of the Requirements for the Degree
Master of Science

Amirhessam Tahmassebi

August, 2015
ABSTRACT

The investigation into the behavior of the fluids in nanoscale channels, such as carbon nanotubes leads us to a new approach in the field of nanoscience. This is referred to as nano-fluidics, which can be used in nano-scale filtering and as nano-pipes for conveying fluids. The behavior of fluids in nano-fluidic devices is very different from the corresponding behavior in microscopic and macroscopic channels. In this study, we investigate the fluid flow through carbon nanotubes and graphene based nanostructures using a molecular dynamics (MD) method at a constant temperature. Three different models were created which contain single-walled carbon nanotube, graphene, and a combination of both. Liquid argon is used as fluid in the system. In the previous investigations, they were considered bombarding the atoms towards the carbon nanotubes like bullets from a gun, and due to the interactions, they lost most of their momentum. Thus, the chance for the atoms to pass through the carbon nanotube was very low. Here, we employed a new approach using a moving graphene wall to push the argon fluid towards the confinements of the systems. By performing this method, we have tried to make a continuum flow to find out how the physical quantities such as, position, velocity, pressure, and energy change when the fluid flow reaches the confinements of the systems.
ACKNOWLEDGEMENTS

Foremost, I would like to express my sincere gratitude to my advisor Dr. Alper Buldum for the continuous support of my Masters study and research, for his patience, motivation, enthusiasm, and immense knowledge. His guidance helped me in all the time of research and the writing of this thesis. I could not have imagined having a better advisor and mentor for my Masters study.

Besides my advisor, I would like to thank the rest of my thesis committee: Dr. Ben Yu-Kuang Hu and Dr. Robbert Mallik for their encouragement, insightful comments, and hard questions.

My sincere thanks also goes to Dr. Jutta Luettmer-Strathmann, for supporting me during these past two years. She led me during my study and helped me to find my future career. She will be my scientist idol forever.

Last but not the least, I would like to thank my parents for giving birth to me and supporting me throughout my life.
TABLE OF CONTENTS

LIST OF TABLES ................................................................. vii
LIST OF FIGURES ................................................................. viii

CHAPTER

I. INTRODUCTION ................................................................. 1

II. MODEL ................................................................. 7

  2.1 Constituents and interactions ............................................. 7
  2.2 Potential and Force ....................................................... 15
  2.3 Units ................................................................. 18

III. METHOD ................................................................. 20

  3.1 Thermodynamical variable ............................................. 20
  3.2 Thermostat .............................................................. 21
  3.3 Mechanical variable ................................................... 21
  3.4 Periodic Boundary Conditions ......................................... 27

IV. RESULTS ................................................................. 29

  4.1 Energy calculation ..................................................... 29
  4.2 Thermodynamical quantities calculations ............................... 31
  4.3 Flow velocities and positions ........................................ 36
4.4 The effect of moving graphene wall ........................................ 59

V. CONCLUSIONS ................................................................. 64

BIBLIOGRAPHY ................................................................. 67
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>The numerical details of the constituents of the three different models.</td>
<td>14</td>
</tr>
<tr>
<td>2.2</td>
<td>Lennard Jones parameters for different possible interactions.</td>
<td>18</td>
</tr>
</tbody>
</table>
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Poiseuille’s law for a circular pipe.</td>
<td>5</td>
</tr>
<tr>
<td>2.1</td>
<td>The chiral vector $C_h$ for SWNT using an infinite graphene plane which shows how to roll up the nanotube defining $a_1$ and $a_2$ [17].</td>
<td>8</td>
</tr>
<tr>
<td>2.2</td>
<td>Single-walled nanotube (SWNT) armchair (10,10) [17].</td>
<td>8</td>
</tr>
<tr>
<td>2.3</td>
<td>Schematic figure of Model-1 containing Single-Walled Carbon Nanotube (SWNT), graphene wall, and argon atoms which demonstrates the Ar-Ar and Ar-C interactions and the position vectors assigned to atoms.</td>
<td>9</td>
</tr>
<tr>
<td>2.4</td>
<td>Model-1, SWNT armchair (10,10) and moving graphene wall. Pink particles represent Argon atoms and the blue ones represent Carbon atoms. Figure (a) demonstrates the starting state of the model, and the figure (b) shows when the MD simulation completed. In addition, figure (c) is the top view of the model, and the figure (d) is the side view of the model.</td>
<td>11</td>
</tr>
<tr>
<td>2.5</td>
<td>Model-2, rigid graphene wall with a hole and moving graphene wall. Pink particles represent Argon atoms and the blue ones represent Carbon atoms which are labeled in the image. The figure (a) demonstrates the starting state of the model, and the figure (b) shows the model when the MD simulation completed. Moreover, the figure (c) shows the side view of the model at the starting point, and the figure (d) pictures the side view of the model when the moving graphene wall reached to the end point after the total MD steps.</td>
<td>12</td>
</tr>
</tbody>
</table>
2.6 Model-3, SWNT armchair(10,10) and the rigid graphene wall including a hole with the same radius of the SWNT which is attached to the mouth of the SWNT, and moving graphene wall. Pink particles represent Argon atoms and the blue ones represent Carbon atoms which are labeled in the image. The figure (a) shows the starting point of the model, and the figure (b) pictures the model when the MD simulation is completed and the moving graphene wall got closer to the rigid graphene wall. In addition, the figure (c) shows the side view of the model at the starting point of the simulation, and the figure (d) demonstrates the model when the MD simulation completed.

2.7 Lennard-Jones potential intermolecular potential energy. $\sigma$ represents the size parameter, and $\epsilon$ represents the energy parameter.

2.8 Lennard-Jones potential intermolecular potential energy indicating the repulsive and attractive parts. $\sigma$ represents the size parameter and $\epsilon$ represents the energy parameter.

3.1 Temperature in reduced units versus MD time steps. The red line demonstrates the development of the temperature over time for Model-1, the green line for Model-2 and the blue one for the Model-3.

3.2 Energy in reduced units versus MD time steps for Model-1. The red points demonstrate the potential energy, the green point-line shows the kinetic energy, and the solid blue line is related to the total energy.

3.3 Energy in reduced units versus MD time steps for Model-2. The red points demonstrate the potential energy, the green point-line shows the kinetic energy, and the solid blue line is related to the total energy.

3.4 Energy in reduced units versus MD time steps for Model-3. The red points demonstrate the potential energy, the green point-line shows the kinetic energy, and the solid blue line is related to the total energy.

3.5 Periodic boundary conditions for a molecular dynamics simulation using a 3-D ($L_x \times L_y \times L_z$) box. The arrows denote atoms and their velocities.

4.1 Development of total energy density (energy/volume) in reduced units for different models over time steps. The green line demonstrates the energy density for Model-1, the red one for Model-2, and the blue line is related to the Model-3.
4.2 The development of the average energy per volume over time for argon fluid through different models. The red solid line demonstrates the average energy and violet lines point shows its error for Model-1, the green solid line shows the average energy and the sky blue lines point pictures its error for Model-2, and the blue solid line pictures the energy and yellow lines point shows its error for the Model-3. All of the energy measurements are in reduced units.

4.3 Average pressure of the inside of the nanotube in reduced unit over time steps for different models. The red line demonstrates the pressure inside the nanotube for Model-1, the blue line shows the pressure along the hole inside the rigid graphene wall over time steps, and the green line depicts the pressure inside the nanotube which has been attached to the graphene wall with a hole at the mouth of the nanotube. All of the pressure measurements are in reduced units.

4.4 The development of the average pressure of the nanotube over time for argon fluid through different models. The red lines point demonstrates the average pressure for Model-1, the green lines point shows the average pressure for Model-2, and the blue ones pictures for the Model-3. All of the pressure measurements are in reduced units.

4.5 Non-dimensional pressure development along the nanotube axis for different models. The red line depicts the pressure versus Z-axis of the nanotube for Model-1, the green line demonstrates the pressure along the Z-axis for Model-2, and the blue line shows the pressure along the Z-axis for Model-3. All of the pressure measurements are in reduced unit and the Z-axis is in angstrom units.

4.6 The non-dimensional pressure along the nanotube axis for different models. Standard deviation has been calculated for each model. The red lines point demonstrates the pressure for the Model-1, the green lines point shows pressure for the Model-2, and the blue one is related to the pressure versus Z-axis for the Model-3. All of the pressure measurements are in reduced units and the Z-axis is in angstrom units.

4.7 The development of z-component of the velocity for the argon flow for Model-1 along the nanotube axis. The velocity measurements are in reduced unit and z-positions are in angstrom units.

4.8 The development of z-component velocity of the argon flow for Model-2 along the hole on the graphene wall (Z-axis). The velocity measurements are in reduced unit and z-positions are in angstrom units.
4.9 The development of z-component velocity of the argon flow for Model-3 along the hole on the graphene wall, and the nanotube (Z-axis). The velocity measurements are in reduced unit and z-positions are in angstrom units. .................................................. 38

4.10 Figure (a) shows the development of the z-components of the velocity along nanotube axis for Model-1. Figure (b) demonstrates the velocity has shown in figure (a) after running average with considering the standard deviation error. .................................................. 40

4.11 Figure (a) shows the development of the z-components of the velocity along nanotube axis for Model-2. Figure (b) demonstrates the velocity has shown in figure (a) after running average with considering the standard deviation error. .................................................. 40

4.12 Figure (a) shows the development of the z-components of the velocity along nanotube axis for Model-3. Figure (b) demonstrates the velocity has shown in figure (a) after running average with considering the standard deviation error. .................................................. 41

4.13 The development of the z-component of the velocity along the nanotube axis. The solid red line demonstrates the $V_z$ versus $Z$ for the Model-1 with violet standard error lines, the green solid line for Model-2 with cyan standard error lines, and the blue solid line shows how fast the argon flow moves through Model-3 with yellow standard error lines. The velocity measurements are in reduced unit, and the positions are in angstrom units. .................................................. 43

4.14 The development of the radial speed over nanotube radius for different three models. The solid red line demonstrates this phenomenon for Model-1, the green one for Model-2, and the blue line shows radial speed versus radius for Model-3. All of the velocity measurements are in reduced unit and nanotube radius has been demonstrated in angstrom units. .................................................. 44

4.15 The top-view of the nanotube in Model-1. The red circles demonstrate the carbon atoms which make single-walled nanotube and green crosses show the argon atoms. Both X and Y positions are in angstrom units. .................................................. 45

4.16 The top-view of the hole on the graphene wall in Model-2. The figure (a) shows the the graphene wall made by carbon atoms showed by red circles and the argon atoms passing through the hole inside the wall indicated by green crosses. Figure (b) demonstrates the flow area deeply. Both X and Y positions are in angstrom units. .................................................. 46
4.17 The top-view of the nanotube and the hole on the graphene wall in Model-3. The figure (a) shows the the graphene wall made by carbon atoms and SWNT are shown by red circles and the argon atoms passing through the SWNT and the hole on the wall are indicated by green crosses. Figure (b) demonstrates the flow area deeply. Both X and Y positions are in angstrom units. 47

4.18 Y-Z trajectory of the Model-1. The figure (a) demonstrates the argon atoms inside an imaginary cylinder with radius $\sim 10A^0$ and length $\sim 20A^0$. Moreover, figure (b) shows the argon flow inside an imaginary cylinder with radius $\sim 8A^0$ and length $\sim 10A^0$. The red plus signs demonstrate the single-walled carbon nanotube, and the green cross signs show the argon atoms. Both measurements are in angstrom units. 49

4.19 Y-Z trajectory of the Model-2. The figure demonstrates the argon atoms inside an imaginary cylinder with radius $\sim 10A^0$ and length $\sim 10A^0$. The red circles demonstrate the rigid graphene wall with a hole and the green cross signs show the argon atoms. Both measurements are in angstrom units. 50

4.20 Y-Z trajectory of the Model-3. The figure (a) demonstrates the whole view of the model with argon atoms inside an imaginary cylinder with radius $\sim 8A^0$ and length $\sim 20A^0$. In figure (b) to show deeper point of view of figure (a) we just considered the region we have the argon atoms. The red circles demonstrate the single-walled carbon nanotube and the graphene sheet, and the green cross signs show the argon atoms. Both measurements are in angstrom units. 50

4.21 Y-Z trajectory of the Model-3. The figure (a) demonstrates the whole view of the model with argon atoms inside an imaginary cylinder with radius $\sim 10A^0$ and length $\sim 20A^0$. In the figure (b) to show a deeper point of view of the figure (a), we just considered the region that we have the argon atoms in. The red circles demonstrate the single-walled carbon nanotube and the graphene sheet, and the green cross signs show the argon atoms. Both measurements are in angstrom units. 52

4.22 X-Y trajectory of the Model-3. The figure demonstrates the cross section view of the model with argon atoms inside an imaginary cylinder with radius $\sim 10A^0$ and length $\sim 20A^0$. The red circles demonstrate the single-walled carbon nanotube and the graphene sheet, and the green cross signs show the argon atoms. Both measurements are in angstrom unit. 53
4.23 Vector plot of the argon flow passing through Model-1. The dashed box has shown the side-view of the SWNT, and the blue arrows demonstrated the direction and speed of the movements of the argon flow through SWNT in Y-Z plane. Both measurements are in angstrom units. ................................................................. 54

4.24 Vector plot of the argon flow passing through Model-2. The dashed box has shown the side-view of the graphene wall, and the blue arrows demonstrated the direction and speed of the movements of the argon flow through SWNT in Y-Z plane. Both measurements are in angstrom units. ................................................................. 55

4.25 Vector plot of the argon flow passing through Model-3. The dashed box has shown the side-view of the SWNT and graphene wall, and the blue arrows demonstrated the direction and speed of the movements of the argon flow through SWNT in Y-Z plane. Both measurements are in angstrom units. ................................................................. 56

4.26 The average X-direction of the argon atoms in each time steps. The red linespoint demonstrates Model-1, the green one Model-2, and the blue linespoint shows the mean value of the X-direction for Model-3. The position measurements are in angstrom unit. ................. 57

4.27 The average Y-direction of the argon atoms in each time steps. The red linespoint demonstrates Model-1, the green one Model-2, and the blue linespoint shows the mean value of the Y-direction for Model-3. The position measurements are in angstrom unit. ................. 57

4.28 The average Z-direction of the argon atoms in each time steps. The red linespoint demonstrates Model-1, the green one Model-2, and the blue linespoint shows the mean value of the Z-direction for Model-3. The position measurements are in angstrom unit. ................. 58

4.29 The average speed of the argon atoms in each time steps. The red linespoint demonstrates Model-1, the green one Model-2, and the blue linespoint shows the mean value of the X-direction for Model-3. The speed measurements are in reduced unit. .................. 59

4.30 Temperature in reduced units versus MD time steps. The red line demonstrates the development of the temperature over time for Model-1, the green line for Model-2 and the blue one for the Model-3. . 60
4.31 The development of the average energy per volume over time for argon fluid through different models. The red solid line demonstrates the average energy and violet line shows its error for Model-1, the green solid line shows the average energy and the sky blue line points its error for Model-2, and the blue solid line pictures the energy and yellow linepoints show its error for the Model-3. All of the energy measurements are in reduced units.

4.32 The development of the average pressure of the nanotube over time for argon fluid through different models. The red linepoint demonstrates the average pressure for Model-1, the green linepoint shows the average pressure for Model-2, and the blue ones pictures for the Model-3. All of the pressure measurements are in reduced units.

4.33 The comparison of average pressure of the nanotube for the models with using different velocity for moving graphene wall. The three red, green, and blue solid lines represent the changing of the average pressure of the nanotube over MD time steps for Model-1, Model-2, and Model-3 respectively. In addition, the three violet, cyan, and yellow linepoints represent the development of the average pressure of the nanotube versus MD time steps for Model-1, Model-2, and Model-3. All of the measurements are in reduced units.
CHAPTER I
INTRODUCTION

The discovery of carbon nanotubes [1] has played an important role in both experimental and computational research in nano-materials science and nanotechnology [2]. In addition to this, behavior of the fluids in nano-scale channels, such as carbon nanotubes created a new field of nano-science. This is referred to as nano-fluidics, which can be used in nano-scale filtering and as nano-pipes for conveying fluids. In the last few years, since the carbon nanotubes are seen as promising biocompatible nanomaterial, fluid technology began arise from different fields, including, e.g., biochemistry, biomedicine, and drug delivery [3].

The behavior of fluids in nano-fluidic devices is very different from the corresponding behavior in microscopic and macroscopic channels [2]. Any objects moving through a fluid (liquid or gas) experiences a drag force opposing its motion. In general, the drag force can be written as:

\[ \vec{F}_{\text{drag}} = -\vec{v} f(v, \rho, \eta, L, \text{shape}) \] (1.1)

Where \( \vec{v} \) is the velocity relative to the fluid, \( \rho \) is the density of the fluid, \( \eta \) is the viscosity of the fluid, \( L \) is the linear dimension of the object (e.g. diameter of the nanotube), and \( f \) is a function of \( v, \rho, \eta, \) and \( L \) which also depends on the shape of
the object (e.g. cylindrical shape of nanotube). To our knowledge, at present, there is no technique used to measure the drag on a nanotube in liquid flow. However, a molecular dynamics simulation method provides a powerful tool to investigate liquid flow at the molecular level [4].

Depending on the circumstances, the drag force can have very different forms. In this regard, we are defining the Reynold’s number $R$ which is a dimensionless quantity that is used to characterize the flow of the fluid around the object. For the circular pipe we have:

$$R = \frac{v \rho L}{\eta}$$

Where $v$ is the velocity of the fluid, $\rho$ is the density of the fluid, $L$ is the diameter of the circular pipe, and $\eta$ is the viscosity of the fluid.

For low Reynold’s number, $R \ll 1$, the flow is laminar (no turbulence) and for large Reynold’s number, $R \gg 1$, the flow is turbulent, and the drag force becomes independent of viscosity and depends only on the density $\rho$ of the fluid, the speed $v$, and size $L$ and the shape of the object. If the diameter of our pipe is small enough, the effect of viscosity is much larger than velocity or density. In other words, liquid which flows freely on the macro scale flows like honey on the nanoscale [5].

Koplik et. al. [6] has answered the questions concerning what boundary conditions satisfy the low Reynold’s number flows at solid surfaces [7]. In order to clarify the ambiguous parts, molecular dynamics simulations of liquid argon as viscous fluid flows past no-slip boundary conditions have been carried out. They have confirmed
that the fluid flow at a microscopic level has appropriate boundary conditions in most of the parts which behave like a continuum fluid in motion.

On the other hand, Tang et. al. [4] has employed nonequilibrium molecular dynamics simulations of models which were created by uniform liquid argon that flow past single and double walled carbon nanotubes to calculate drag force. Comparing the results to the drag coefficient for flows calculated through Navier-Stokes equations [8] and with help of finite element methods has led them to the point that the drag on a nanotube cannot be solved due to the classical continuum mechanics.

In addition, Falk et. al. [9] has tried to present a theoretical approximation for the friction coefficient. Using molecular dynamics flow simulations of water, ethanol, and decane through graphitic nanopores, they have shed light on the point that friction between liquids and confinements depends on the geometries of the nanopores. In order to support the previous experimental investigations, flow velocities of different liquids were exhibited.

The molecular dynamics simulations of argon-filled single walled carbon nanotubes under high pressure have been performed by Shanavas et. al. [10] to inquire the phase transition with the help of the Raman [11] spectroscopy method. Collapsing carbon nanotubes to ribbon like structures at low pressure has been reported. They also have deduced that the peak position depends linearly on frequency and tube diameter [12].

Tuzun et. al. [13] has performed molecular dynamics simulations of the flow of helium and argon inside carbon nanotubes of several sizes. They have came up
with the fact that the behavior of the fluid strongly depends on the rigidity of the tube, fluid density, and tube diameter. They also have understood the behavior of the fluid does not depend on the length of the nanotube; however, the dynamics of the nanotube have played an important role in this regard. They have shown that dynamic nanotubes slowed down the fluid more than the fixed nanotubes.

In this work, a new approach is used for the modeling and simulation of fluid flow through nanostructures. The previous modeling and simulation efforts were based on the dissemination of the atoms or molecules which were hurled to the carbon channels with assigned initial velocities. Here, three different models which contain combinations of carbon nanotube and graphene wall which were embedded in liquid argon. The argon liquid was pushed by moving a graphene wall with a constant velocity. By taking this into account, we present a new approach of the modeling in comparison to the previous models in which the atoms were shot like bullets from a gun at carbon nanotubes. On the other hand, by pushing the atoms through the moving graphene wall toward the carbon nanotube, the atoms have the ability to go through the carbon nanotube, despite the previous models in which the atoms lost their momentum after shooting in the middle of the way. In other words, the chance to get through to nanotube was low.

According to Poiseuille’s law [14] for flow rate in a circular pipe, we have:

$$\Delta P = \frac{8\eta LQ}{\pi r^4} \quad (1.3)$$
Where $\Delta P$ is pressure drop, $\eta$ is dynamic viscosity, $L$ is the length of the nanotube, $Q$ is volumetric flow rate, and $r$ is the radius of the nanotube.

![Diagram of Poiseuille's Law](image)

**Figure 1.1: Poiseuille's law for a circular pipe.**

Due to the difference in length scale, continuum theories for macroscale flow may break down when considering similar flows at nanoscale [4]. As we have seen, the pressure drop is proportional to $r^{-4}$, which means at nanoscales with nano-ranges of tube radii, it is hard to overcome the flow rate and push the fluid through nanotubes. This study aims to investigate the flow rate in our nanoscale models with radius $\sim 6.1A^0$ and length $\sim 130A^0$ with a new approach which involved the atoms pushing continuously via the moving graphene wall. In the section 4.4, we also investigate the effect of the velocity of the moving graphene wall on the systems. We study the development of the pressure, energy, velocity, and positions of the fluid flow inside and outside of the nanotube over MD time steps, and in some cases, we find the rate...
of change of these quantities along the direction of the nanotube axis. We found that the argon flow has taken a different position in model, which contains nanotube in comparison to the model contains graphene wall. We also study the variations of the velocity along the nanotube.

The outline of this thesis is as follows: In chapter 2 we introduce the models containing constituents and interactions. In chapter 3 we describe the simulations methods with the help of introducing the mechanical and thermodynamical variables. We present our results in chapter 4 and end with conclusions in chapter 5.
CHAPTER II

MODEL

In our simulation we used three different models containing single-walled carbon nanotube, moving graphene wall, and argon atoms flowing through the system, which is discussed in section 2.1. In this work, we used $\sigma_{Ar-Ar}$ as the unit of length, $\epsilon_{Ar-Ar}$ as the unit of energy, and $m_{Ar}$ (atomic mass of argon) as the unit of mass. The relation among physical parameters is discussed in section 2.2 respectively.

2.1 Constituents and interactions

Carbon nanotubes (CNT) are allotropes of carbon which have tubular cylindrical shape [16]. All carbon nanostructures have one atom in the wall thickness and tens of atoms around the perimeter with typical diameters around 1.4nm. In fact, the planar sheets are rolled at a determined angle which are called chiral angles. Nanotubes are known as a member of fullerene structural family which categorized to single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs).

The SWNTs can be defined using the vector $C_h$ [15].

$$C_h = na_1 + ma_2$$ (2.1)
When the numbers $n$ and $m$ are equal to each other, we have the case armchair for the nanotube. This numbers mean the number of carbon atoms in chiral angle. Our model consists of an armchair$(10,10)$ which is shown in the picture below (see Figure 2.2).

Figure 2.1: The chiral vector $C_h$ for SWNT using an infinite graphene plane which shows how to roll up the nanotube defining $a_1$ and $a_2$ [17].

Figure 2.2: Single-walled nanotube (SWNT) armchair $(10,10)$ [17].
In this study we used three different models which included the carbon nanotubes and graphene wall. We also used argon atoms to study the flow through the carbon nanotube, graphene wall with hole biased by moving graphene wall. We set the carbon atoms of the SWNT and the graphene wall with hole rigid (fixed), so there is no interaction among these carbon atoms. We have interaction among argon atoms and the carbon atoms and definitely an interaction among argon atoms with themselves. In other words, we are dealing with Ar-C and Ar-Ar interactions in this simulation and by fixing the coordinates of carbon atoms, we won’t have any C-C interaction at all.

Figure 2.3: Schematic figure of Model-1 containing Single-Walled Carbon Nanotube (SWNT), graphene wall, and argon atoms which demonstrates the Ar-Ar and Ar-C interactions and the position vectors assigned to atoms.
As I mentioned before, we studied three different models and here I’m going to explain every model in details.

2.1.1 Model-1

For the model-1 we simulate a three dimension box \((X = 56.57A^0, Y = 55.38A^0, Z = 129.65A^0)\) with a SWNT armchair \((10,10)\) with \((X_{\text{Origin}} = 27.13A^0, Y_{\text{Origin}} = 26.26A^0, L = 47.96A^0, R = 6.1A^0)\), a moving graphene wall which starts from the end of the box \((Z = 129.65A^0)\) with velocity \((\frac{0.05A^0}{1000Timestep} \sim 18A^0\mu s)\) towards the mouth of the nanotube, and argon atoms which flow through the carbon nanotube (see Figures below).
2.1.2 Model-2

For the model-2 we simulate a three dimension box \((X = 56.57\,\text{Å}, Y = 55.38\,\text{Å}, Z = 129.65\,\text{Å})\) with a plane of carbon at \((Z = 47.96\,\text{Å})\) which has a hole with radius \((X_{\text{Origin}} = 27.13\,\text{Å}, Y_{\text{Origin}} = 26.26\,\text{Å}, R_{\text{Hole}} = 6.1\,\text{Å})\) which has the same radius of the nanotube we defined in the model-1, a moving graphene wall which starts from the end of the box \((Z = 129.65\,\text{Å})\) with velocity \((\frac{0.05\,\text{Å}}{1000\,\text{Timestep}} \sim 18\,\frac{\text{Å}}{\text{µs}})\) towards the hole on the rigid graphene wall and argon atoms likewise the model-1 (see Figures below).
Figure 2.5: Model-2, rigid graphene wall with a hole and moving graphene wall. Pink particles represent Argon atoms and the blue ones represent Carbon atoms which are labeled in the image. The figure (a) demonstrates the starting state of the model, and the figure (b) shows the model when the MD simulation completed. Moreover, the figure (c) shows the side view of the model at the starting point, and the figure (d) pictures the side view of the model when the moving graphene wall reached to the end point after the total MD steps.
2.1.3 Model-3

In this model, we combined the previous two models together. We have a SWNT armchair (10,10) with \( X_{\text{Origin}} = 27.13 \text{Å}, Y_{\text{Origin}} = 26.26 \text{Å}, L = 47.96 \text{Å}, R = 6.1 \text{Å} \) and we put the plane of carbon atoms (rigid graphene wall), which has a hole we already defined in model-2 with the same radius as the radius of the SWNT at the end of the mouth of the SWNT, a moving graphene wall which starts from the end of the box \( Z = 129.65 \text{Å} \) with velocity \( \frac{0.05 \text{Å}}{1000 \text{Timestep}} \sim 18 \frac{\text{Å}}{\text{µs}} \) towards the hole on the rigid wall, and the argon atoms which play the flow of the system (see figures below).
Figure 2.6: Model-3, SWNT armchair(10,10) and the rigid graphene wall including a hole with the same radius of the SWNT which is attached to the mouth of the SWNT, and moving graphene wall. Pink particles represent Argon atoms and the blue ones represent Carbon atoms which are labeled in the image. The figure (a) shows the starting point of the model, and the figure (b) pictures the model when the MD simulation is completed and the moving graphene wall got closer to the rigid graphene wall. In addition, the figure (c) shows the side view of the model at the starting point of the simulation, and the figure (d) demonstrates the model when the MD simulation completed.

<table>
<thead>
<tr>
<th>Model No.</th>
<th>No. of atoms</th>
<th>No. of C</th>
<th>No. of Ar</th>
<th>SWNT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model-1</td>
<td>5124</td>
<td>1996</td>
<td>3128</td>
<td>$L = 47.96A^0, R = 6.1A^0$</td>
</tr>
<tr>
<td>Model-2</td>
<td>5448</td>
<td>2339</td>
<td>3109</td>
<td>N/A</td>
</tr>
<tr>
<td>Model-3</td>
<td>5020</td>
<td>3120</td>
<td>1900</td>
<td>$L = 47.96A^0, R = 6.1A^0$</td>
</tr>
</tbody>
</table>

Table 2.1: The numerical details of the constituents of the three different models.
2.2 Potential and Force

The potential energy of each model is the sum over all of the contributions of the constituents of the system which we defined before and depends on the position.

\[ U = U(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) \] (2.2)

Where the \( N \) is the total number of particles and \( \vec{r}_i \) is the position of the particle \( i \). In addition, we know how to calculate the conservative force from the potential energy using the negative gradient of the potential energy with respect to the position particle \( i \).

\[ \vec{F}_i = -\nabla_i U(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) \] (2.3)

2.2.1 Lennard-Jones Potential

The Lennard-Jones potential is a simple model that approximates the interaction between a pair of neutral atoms or molecules [18].

\[
V_{LJ} = \begin{cases} 
4\epsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} & \text{if } r < r_{cut} \\
0 & \text{if } r > r_{cut}
\end{cases}
\] (2.4)

With \( r \) which is the distance between particles, \( \epsilon \) which is the depth of the potential and has the energy unit, and \( \sigma \) which is the size parameter and determines the closest distance among the particles and where the inter-particle potential is zero and \( r_{cut-off} = 2.5\sigma \) (see Figure 2.7).
Moreover, we can calculate the inter-particle force as we mentioned before,

$$\vec{F}_{ij} = 48 \frac{\epsilon}{\sigma^2} \left[ \left( \frac{\sigma}{r} \right)^{13} - \frac{1}{2} \left( \frac{\sigma}{r} \right)^{7} \right] \left( \vec{r}_i - \vec{r}_j \right)$$

(2.5)

Which would be attractive for $r > r_{min} = 2^{\frac{1}{6}} \sigma$ and repulsive for $r < r_{min} = 2^{\frac{1}{6}} \sigma$ (see Figure 2.8).
Figure 2.8: Lennard-Jones potential intermolecular potential energy indicating the repulsive and attractive parts. $\sigma$ represents the size parameter and $\epsilon$ represents the energy parameter.

With rigid nanotube models, only Lennard-Jones potentials between argon atoms and between carbon and argon pairs need to be considered in the simulations. Therefore, we are just dealing with two kinds of inter-particle interactions Ar-Ar and Ar-C, and using Lorentz-Berthelot [19] mixing rules we have:

\[
\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \tag{2.6}
\]

\[
\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j} \tag{2.7}
\]
We performed three different models to simulate the interaction of Argon atoms through the combination of the SWNT and moving graphene wall. In the code, non-dimensional parameters or [reduced molecular dynamics (MD)] units were used by choosing $\sigma_{Ar-Ar}$, $\epsilon_{Ar-Ar}$, and $m_{Ar}$ (atomic mass of argon) as the units of length, energy, and mass. Respectively, we set the unit for the energy to $\epsilon$ and the reduced temperature $T^* = \frac{k_b}{\epsilon}T = 0.97K$. Since, we simulated the liquid Argon fluid at 85K with a density $1342Kg/m^3$ and a dynamic viscosity of $2084 \times 10^{-7}kg/ms$, using boltzman constant $k_b = 1.3806488 \times 10^{-23}m^2kgs^{-2}K$. We have also calculated the pressure in reduced unit $P^* = \frac{\sigma^2}{\epsilon}P$.

The other conversion is the unit of the time which we derived it from mass, size, and energy units, $[t] = \sqrt{\frac{|M|\sigma^2}{\epsilon}}$ which the mass of Argon is $M = 6.6 \times 10^{-26}kg$,

<table>
<thead>
<tr>
<th>Interaction/Parameters</th>
<th>$\sigma [A^0]$</th>
<th>$\epsilon [J]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Argon-Argon</td>
<td>3.8388</td>
<td>$1.209846 \times 10^{-21}$</td>
</tr>
<tr>
<td>Argon-Carbon</td>
<td>3.573</td>
<td>$1.9646 \times 10^{-21}$</td>
</tr>
</tbody>
</table>

Table 2.2: Lennard Jones parameters for different possible interactions.

2.3 Units
yields us to $\delta t = 2.83 \times 10^{-12} \text{s}$ with simulating about $1.2 \times 10^6$ steps which will come up with $3.396 \times 10^{-6} \text{s} \simeq 3.4 \mu \text{s}$.
CHAPTER III

METHOD

3.1 Thermodynamical variable

We represent our models with respect to the canonical ensemble in statistical mechanics when the possible state of the mechanical system is in thermal equilibrium with a heat bath at some fixed temperature. In fact, the system can exchange energy with a heat bath and what fluctuates here is the energy over time. Our ensemble typically depends on the absolute temperature $T$, number of particles in the system $N$, and the system’s volume $V$. In statistical mechanics, an ensemble with these parameters is called $NVT$ ensemble too [20]. The ensemble is obtained by controlling the temperature through direct temperature scaling during the data collection phase at initialization stage by means of temperature-bath. For this procedure we used a thermostat which we will talk about in details in section 3.2. For defining pressure, volume, and density we should use periodic boundary conditions which we discuss it in the section 3.4.
3.2 Thermostat

Since we are dealing with NVT ensemble, and interested in the behavior of the system at a fixed temperature, a thermostat to control the temperature at a constant number is required. The other reason we used a thermostat is to avoid steady energy drifts caused by the accumulation of numerical errors during MD simulation. The easiest algorithm to keep the temperature constant is the velocity re-scaling [23]. If the temperature at time $t$ is $T(t)$ and the velocities are multiplied by a factor $\lambda$, then the associated temperature change can be calculated as:

$$\Delta T = \frac{1}{2} \sum_{i=1}^{N} \frac{2}{3} \frac{m_i (\lambda v_i)^2}{N k_B} - \frac{1}{2} \sum_{i=1}^{N} \frac{2}{3} \frac{m_i v_i^2}{N k_B}$$ (3.1)

where $\lambda = \sqrt{\frac{T_{\text{new}}}{T(t)}}$. So, in each MD time step we are going to multiply all of the velocities by a factor $\lambda$, and due to this factor we can find the desired temperature which is $T_{\text{new}}$ in our formulation.

3.3 Mechanical variable

To consider the mechanical approach for the studying of multiparticle systems and simulating the dynamics of our system using microscopic equations of motion, we chose Molecular Dynamic (MD) method. The essential idea is using Newton’s second law to calculate positions and velocities of all of the molecules in the system as a
function of time. Since we have a box containing argon atoms, which have the role of the flow of the system colliding into carbon atoms, we should first make sure about the classical limit of the problem. We know that the electrons of the argon atoms are bound to the nuclei, and the energy to send one electron to the exciting level is of order 10 electron volts (eV). This is fairly larger than the kinetic energy of the center of mass of the argon atoms at room temperature (0.1 eV). So, we can conclude that this difference in energy cannot affect the configuration of the argon atoms at all at this temperature. Moreover, we know that the argon atoms with DeBroglie wavelength about $10^{-7} \text{Å}$ never get closer than $1 \text{Å}$, therefore using Newton’s second law would be a good approximation to solve the equations of motion to find the positions and velocities of the atoms as a function of time. In other words, the DeBroglie wavelength which is much smaller than the atomic spacing leads us the classical approach of our system [21].

\[
\vec{F}_{i,j} = m \vec{a}_{i,j}
\]  

(3.3)

Where \(\vec{F}\) is the conservative force due to the Lennard-Jones potential, and \(i = 1, 2, 3, \ldots, N\) is the number of atoms and \(j = x, y, z\) which are our coordinate components. In fact, each particle experiences a force from the other particles due to the collision. For large separation, the interaction of argon atoms is due to the Van der Waals force, which is a weak attraction and varies as \(r^{-6}\) and if the atoms get closer they experience a repulsive force which varies as \(r^{-12}\). The background of the force comes from the transient electric dipole moment and the overlapping of the electron
clouds of two argon atoms. Hence, the velocity is the time derivative of the position and acceleration is the time derivative of the velocity:

\[
\begin{align*}
\dot{a}_{i,x} &= \frac{dv_{i,x}}{dt} \\
v_{i,x} &= \frac{dx_i}{dt} \\
\dot{a}_{i,y} &= \frac{dv_{i,y}}{dt} \\
v_{i,y} &= \frac{dy_i}{dt} \\
\dot{a}_{i,z} &= \frac{dv_{i,z}}{dt} \\
v_{i,z} &= \frac{dz_i}{dt}
\end{align*}
\]

(3.4)

(3.5)

(3.6)

Where \(a_{i,x}, a_{i,y}, \text{ and } a_{i,z}\) are the components of the acceleration \(\vec{a}\) of the \(i\)th particle with the velocities \(v_{i,x}, v_{i,y}, \text{ and } v_{i,z}\) which is located at \((x_i, y_i, z_i)\) in our coordination system. As we have seen, in MD simulation, we are dealing with the differential equations which should be solved using numerical methods. We have a lot of choices to solve these differential equations numerically. Hence, as our MD computation contains a large number of time steps \(\sim 10^6\) and in order to stay away from big errors using Euler method, we are interested in using Verlet algorithm. Likewise, the other numerical methods for solving differential equations, time is a discrete variable that may be labeled by an integer, say \(k\). Verlet method helps us to solve Newton’s equation of motion with a numerical (finite difference) algorithm to go from time \(t_k\) to time \(t_{k+1} = t_k + \delta t\), where \(\delta t\) is the the step size. Since all of the finite difference methods are based on Taylor expansions of the coordinates, for simplicity, we focus on
the $x$-components ($y$ and $z$ components are analogous), drop the particle subscripts and write $x(t)$ for the position at time $t$, and $v(t)$ and $a(t)$ for the corresponding velocity, and acceleration at time $t$, respectively.

$$x(t + \delta t) = x(t) + \frac{dx}{dt}|_{t} \delta t + \frac{1}{2!} \frac{d^2x}{dt^2}|_{t} (\delta t)^2 + \frac{1}{3!} \frac{d^3x}{dt^3}|_{t} (\delta t)^3 + O((\delta t)^4) \tag{3.7}$$

$$x(t + \delta t) = x(t) + v(t)\delta t + \frac{1}{2} a(t)(\delta t)^2 + \frac{1}{3!} \frac{d^3x}{dt^3}|_{t} (\delta t)^3 + O((\delta t)^4) \tag{3.8}$$

If we re-write the equation (3.8) for $-\delta t$, we have:

$$x(t - \delta t) = x(t) - v(t)\delta t + \frac{1}{2} a(t)(\delta t)^2 - \frac{1}{3!} \frac{d^3x}{dt^3}|_{t} (\delta t)^3 + O((\delta t)^4) \tag{3.9}$$

If we add equations (3.8) and (3.9), it is obvious that the odd terms would cancel out and when we solve for $x(t + \delta t)$, we have:

$$x(t + \delta t) = 2x(t) - x(t - \delta t) + a(t)(\delta t)^2 + O((\delta t)^4) \tag{3.10}$$

Which is the basis for the Verlet algorithm. Note that the velocity does not appear in equation (3.10) and we approximate the velocity. To recapitulate:

$$\begin{cases} x_{\text{new}} = 2x - x_{\text{old}} + a_x(\delta t)^2 \\ v_x = \frac{x_{\text{new}} - x_{\text{old}}}{2\delta t} \end{cases} \tag{3.11}$$
Where $x = x(t_k)$, $x_{old} = x(t_k - \delta t)$, $x_{new} = x(t_k + \delta t)$, $v_x = v_x(t_k)$, and $a_x = a_x(t_k)$.

The Verlet algorithm is not self starting and it requires information about two time steps and the initial condition gives information about a single time step [21].

Since in our simulation we are using periodic boundary conditions, the positions have to be corrected after step three. In this regard, we use an Euler-Cromer algorithm to advance the system two time steps from the initial state $x_0$ and $v_0$.

It is always a good idea to monitor the quantities that are expected to be conserved. Since we have (N,V,T) ensemble, we expect to see the temperature is constant over time steps in our simulation in order to recognize when the algorithm/parameters lead to systematic errors.

![Figure 3.1: Temperature in reduced units versus MD time steps. The red line demonstrates the development of the temperature over time for Model-1, the green line for Model-2 and the blue one for the Model-3.](image)
Since, our models are big enough \( \sim 5000 \) atoms, we reached a thermodynamical equilibrium which is an interesting point of our simulation.

Figure 3.2: Energy in reduced units versus MD time steps for Model-1. The red points demonstrate the potential energy, the green point-line shows the kinetic energy, and the solid blue line is related to the total energy.
Figure 3.3: Energy in reduced units versus MD time steps for Model-2. The red points demonstrate the potential energy, the green point-line shows the kinetic energy, and the solid blue line is related to the total energy.

Figure 3.4: Energy in reduced units versus MD time steps for Model-3. The red points demonstrate the potential energy, the green point-line shows the kinetic energy, and the solid blue line is related to the total energy.

3.4 Periodic Boundary Conditions

We simulate our models in a 3-dimensional box with walls at \([X = 0, L_x); (Y = 0, L_y); (Z = 0, L_z)]\) and we have thousands of atoms colliding with each other and the walls. In small systems simulated with tens of atoms, the collision with walls has a significant fraction of the total collision. On the contrary, in our simulation, the
collision of atoms with each other dominates the collision of atoms with the walls. In this regard, it is common to use the periodic boundary conditions (see Figure 3.5).

![Figure 3.5: Periodic boundary conditions for a molecular dynamics simulation using a 3-D \((L_x \times L_y \times L_z)\) box. The arrows denote atoms and their velocities.](image)

As we have seen we have a 3-dimensional box with walls at \([X = 0, L_x]; (Y = 0, L_y); (Z = 0, L_z)\]. The periodic boundary conditions tell us when an atom of argon encounters a wall, it is transported instantly to the opposite side of the box. This trick helps us to avoid all collisions with walls since there are no walls actually in our model.
CHAPTER IV
RESULTS

4.1 Energy calculation

As we have seen in the last chapter, we calculated the potential energy, kinetic energy, and the total energy which is the sum of them for each time steps. We did find the average of the total energy per unit volume which demonstrates the energy density for each model over time steps. In NVT ensemble, we let the energy fluctuate; however, we got thermal equilibrium over time due to the number of particles of the system, which is big enough to have this condition.
Figure 4.1: Development of total energy density (energy/volume) in reduced units for different models over time steps. The green line demonstrates the energy density for Model-1, the red one for Model-2, and the blue line is related to the Model-3.

For having a better understanding of this figure, we divided up the time steps into twelve blocks and found the average energy and standard deviation of the energy in each block for all of the models. We put all of the data in the figure below.

Figure 4.2: The development of the average energy per volume over time for argon fluid through different models. The red solid line demonstrates the average energy and violet lines point shows its error for Model-1, the green solid line shows the average energy and the sky blue lines point pictures its error for Model-2, and the blue solid line pictures the energy and yellow lines point shows its error for the Model-3. All of the energy measurements are in reduced units.
4.2 Thermodynamical quantities calculations

As we have seen before, we kept the temperature constant over time. Thus, we obtained the so-called \((N, V, T)\) canonical ensemble which the total number of particles, the volume of the system, and the absolute temperature are constant over the time. The thermodynamical quantities such as energy and pressure can fluctuate over the time. However, those are meaningful only when the system reaches the equilibrium. In fact, the pressure is the first-order equilibrium thermodynamic properties which is in the thermodynamical limit independent of the statistical ensemble used. According to ergodic hypothesis, if a microscopic variable takes instantaneous values, we should use the time average of that variable. The thermodynamical temperature \(T\) is related to average kinetic energy of the system due to the equipartition theorem [22].

\[
\left\langle \frac{1}{2} \sum_{i=1}^{N} \frac{p_i^2}{m_i} \right\rangle_t = \langle E_{\text{kinetic}} \rangle_t = \frac{3}{2} N k_B T \tag{4.1}
\]

Where the \(k_B\) is the boltzman’s constant and \(3N\) is the number of degrees of freedom in the systems. Since the velocity has three components, we have 3 for each atom which the total would be \(3N\).

In addition, the thermodynamic pressure \(P\) is related to temperature \(T\), volume \(V\) and the Virial internal energy \(U_{\text{Virial}}\). Therefore, we came up with:

\[
P = \langle P_{\text{instantaneous}} \rangle_t = \frac{2E_{\text{kinetic}}}{3V} + \frac{U_{\text{Virial}}}{V} \tag{4.2}
\]
Which the instantaneous pressure depends on the fluctuations of the potential energy $U$ with respect to the volume $V$.

\[
P = \langle P_{\text{instantaneous}} \rangle_t = -\frac{\partial F}{\partial V} = \frac{2E_{\text{kinetic}}}{3V} - \frac{\partial U}{\partial V} \tag{4.3}
\]

Which for the local hydrostatic pressure we have:

\[
P = -\frac{\partial F}{\partial V} = -\frac{1}{3V} \sum_{i<j} r_{ij} f_{ij}(r_{ij}) \tag{4.4}
\]

Where $f_{ij}$ is the inter-particle conservative force due to the LJ potential and $F$ is the Helmholtz free energy [22].
Figure 4.3: Average pressure of the inside of the nanotube in reduced unit over time steps for different models. The red line demonstrates the pressure inside the nanotube for Model-1, the blue line shows the pressure along the hole inside the rigid graphene wall over time steps, and the green line depicts the pressure inside the nanotube which has been attached to the graphene wall with a hole at the mouth of the nanotube. All of the pressure measurements are in reduced units.

For having a better understanding, we divided up the time steps into twelve blocks and found the average pressure and standard deviation of the pressure in each block for all of the models. We put all of the data in the figure below.

![Graph showing average pressure development over time for different models with error bars]

Figure 4.4: The development of the average pressure of the nanotube over time for argon fluid through different models. The red lines point demonstrates the average pressure for Model-1, the green lines point shows the average pressure for Model-2, and the blue ones pictures for the Model-3. All of the pressure measurements are in reduced units.
Figure 4.5: Non-dimensional pressure development along the nanotube axis for different models. The red line depicts the pressure versus Z-axis of the nanotube for Model-1, the green line demonstrates the pressure along the Z-axis for Model-2, and the blue line shows the pressure along the Z-axis for Model-3. All of the pressure measurements are in reduced unit and the Z-axis is in angstrom units.
Figure 4.6: The non-dimensional pressure along the nanotube axis for different models. Standard deviation has been calculated for each model. The red lines demonstrate the pressure for the Model-1, the green lines show pressure for the Model-2, and the blue one is related to the pressure versus Z-axis for the Model-3. All of the pressure measurements are in reduced units and the Z-axis is in angstrom units.

When the pressure is positive, it means the argon fluid is being compressed and wants to expand. When we take a look at figure (4.5), it is clear in the interval $[50\,\text{A}^0 : 85\,\text{A}^0]$ which wall has moved, we have the most compressed argon fluid and behind this interval to the end of the box, the pressure would be dropped. In fact, when the pressure is negative, it means the fluid has expanded and wants to contract. Since the length of the nanotube is $47.96\,\text{A}^0 \sim 50\,\text{A}^0$, the interval $[0 : 50\,\text{A}^0]$ corresponds to the pressure inside of the nanotube especially for the Model-1 and Model-3 and the pressure through the hole of the rigid graphene sheet for the Model-2. According to the figure (4.5), for the Model-1 which has shown with red line, the pressure of the fluid when it reached the mouth of the nanotube has increased and it goes up by factor 2. On the other hand particularly, for the Model-2, when the pressure of the fluid wants to go through the hole, it is dropped a little bit and continued with a constant number. Not surprisingly, the Model-3, which is the combination of the last two models, obeys the rules of the previous models. When the fluid reached the graphene wall and nanotube, we have a huge drop in the pressure since to go through is the carbon nanotube. This result leads us to this point, when the fluid forces go through a narrower tunnel, the pressure drops and it continues at the constant
value. In addition to this, according to the Model-2, since all of the fluid should pass through the hole on the graphene wall and after that, the fluid can expand, but in the Model-3 since the fluid which passed the hole on the graphene wall and confined in the nanotube, the pressure expanded and wanted to contract. That is why we have negative pressure for the Model-3 inside the nanotube. For the SI units we could have 
\[ P = \frac{\epsilon}{\sigma} P^* = 0.02138 \times 10^9 P^* \] in pascal unit. We could say the the pressure inside the nanotube for Model-1 is about 15Gp, for Model-2 is about 4Gp, and for Model-3 is about 2.5Gp.

4.3 Flow velocities and positions

As we know, in molecular dynamics method, we can achieve the position and velocity of each of the constituents of the system as determined at time \( t \). Using this character of MD, the rate of the changing the velocity of the flow in system (argon atoms) inside and outside of the nanotube for the different three models has been investigated. For demonstrating the result, we chose all of the argon atoms for the outside of the nanotube, and when they reach the mouth of the nanotube \( \sim 50A^0 \), we just considered the velocity of the atoms inside the nanotube. For the better understanding, we made figures for the velocity of the atoms along the nanotube axis.
Figure 4.7: The development of z-component of the velocity for the argon flow for Model-1 along the nanotube axis. The velocity measurements are in reduced unit and z-positions are in angstrom units.
Figure 4.8: The development of z-component velocity of the argon flow for Model-2 along the hole on the graphene wall (Z-axis). The velocity measurements are in reduced unit and z-positions are in angstrom units.

Figure 4.9: The development of z-component velocity of the argon flow for Model-3 along the hole on the graphene wall, and the nanotube (Z-axis). The velocity measurements are in reduced unit and z-positions are in angstrom units.

The moving graphene wall starts moving after 100000 MD time steps with velocity \( \left( \frac{0.05 A^0}{1000 \text{ Timestep}} \right) \sim 18 \frac{A^0}{\mu s} \). The reason of the gap about 65\( A^0 \) – 75\( A^0 \) is that the moving graphene wall has stopped in this region. Thus, we don’t have argon atoms about this wall. All of the atom’s velocities beyond the nanotube \( \sim 50 A^0 \) have been considered, and once after this region, we have considered the atoms inside the nanotube and their velocities respectively. That is why the number density of the
atoms inside the nanotube is lower than the compression of the atoms outside of the nanotube. For the Model-2, it is obvious along the axis of the region which moving graphene wall has stopped, we have more fluctuations than Model-1, instead of the nanotube we used in Model-1, we put a rigid graphene wall with a hole with the same radius of the nanotube. So, the flow has been blocked by the rigid graphene wall and the only way to pass through the wall is the hole. So, the number density of the argon atoms after passing through the wall would be lower. If we go deeper, we will see that the flow velocity inclined to stop when it reached the nanotube. In other words, we have a drop immediately after passing through the nanotube. In Model-2 and Model-3, that would appear as obvious, since the flow has been blocked by the rigid graphene wall. In fact, most of the argon atoms lost their momentum after colliding into the graphene wall and there is not much enough energy and velocity to pass through the nanotube respectively. So, the flow velocity dropped when reached the confinements. For better understanding of this phenomenon, we divided up the z-axis into some blocks, took the average velocity through these blocks, and replotted the results. For having meaningful results, we found the standard deviation error in each block too.
Figure 4.10: Figure (a) shows the development of the $z$-components of the velocity along nanotube axis for Model-1. Figure (b) demonstrates the velocity has shown in figure (a) after running average with considering the standard deviation error.

Figure 4.11: Figure (a) shows the development of the $z$-components of the velocity along nanotube axis for Model-2. Figure (b) demonstrates the velocity has shown in figure (a) after running average with considering the standard deviation error.
Figure 4.12: Figure (a) shows the development of the z-components of the velocity along nanotube axis for Model-3. Figure (b) demonstrates the velocity has shown in figure (a) after running average with considering the standard deviation error.

When we take a look at these graphs, it is clear when we are dealing with a rigid graphene wall in our models. We have a drop after the wall for the velocities. We employed a moving graphene wall to increase the chance of the flow to pass through the hole and nanotube by making a continuum flow because of the momentum made by the moving graphene wall. Since the previous researchers used to employ bombardment the atoms towards the nanotube and most of the atoms lost their momentum and the chance of getting through the confinements was about zero. Most of them did research on the nanotube and they did not put the rigid graphene wall with a hole under investigation [13]. That is the point of the treatment of the flow near the hole of the rigid graphene wall has been investigate. As we have shown in our figures, when the flow reaches the graphene wall, it has been blocked by the
moving graphene wall and the rigid graphene wall and the only way to escape this condition is by passing through the hole in Model-2 and respectively getting through the mouth of the nanotube attached to the rigid graphene wall in Model-3. Because of this situation, the argon atoms which play the role of the flow of the system are trapped in the region between $50A^0 - 60A^0$. They did have interactions with the walls and the other argon atoms. Thus, they lost most of their momentum which was gained through the moving graphene wall when they traversed the length of the nanotube until that region and just a few argon atoms had the chance to pass through the hole. Therefore, the velocity of the argon atoms at $50A^0$ dramatically dropped and when we took the average of the velocities which are shown as figures (b), the slope of the lines after confinements is negative. On the other hand, for Model-1 the slope of the velocity inside the nanotube is positive. To conclude, it seems when we have a rigid graphene wall with a hole in our models, it helps us to control the velocity of the flow and makes it slower. Moreover, having a nanotube in our model depends on the other confinements effect too. In other words, the effect of the rigid graphene wall on the velocity is much more than nanotube. So, if we combine both of the together in a model like Model-3, the graphene wall plays an important role to change the rate of the flow and the nanotube usually obeys that rules. We put all of this data together in one graph with standard deviation calculated in some blocks for each model.
Figure 4.13: The development of the z-component of the velocity along the nanotube axis. The solid red line demonstrates the $V_z$ versus $Z$ for the Model-1 with violet standard error lines, the green solid line for Model-2 with cyan standard error lines, and the blue solid line shows how fast the argon flow moves through Model-3 with yellow standard error lines. The velocity measurements are in reduced unit, and the positions are in angstrom units.

Using a moving graphene wall helped us to increase the momentum of the argon atoms constantly to have a continuum flow. Despite the previous simulations which they unleashed, the argon atoms like bullets from the gun and in the middle of the way when they reach the confinement of the system such as, hole or nanotube, they lost most of their momentum and consequently their velocities decrease. Although, it is hard to put under consideration the treat of the flow inside the nanotube, we used this method to find out the better approach inside the nanotube.
To see this phenomenon inside the nanotube more deeply, we found the rate of changing of the radial speed $V_{radial} = \sqrt{V_x^2 + V_y^2}$ over the radius of the nanotube $\sim 6.1A^0$.

![Figure 4.14](image)

Figure 4.14: The development of the radial speed over nanotube radius for different three models. The solid red line demonstrates this phenomenon for Model-1, the green one for Model-2, and the blue line shows radial speed versus radius for Model-3. All of the velocity measurements are in reduced unit and nanotube radius has been demonstrated in angstrom units.

According to this figure, we have observed that the fluid flow likes to pass through a determined part of the nanotube. For the Model-1 and Model-3, which the models contain nanotube, the argon atoms inclined to get through about the radius $\sim 3A^0 - 4A^0$ from the origin of the nanotube. Nevertheless, for the Model-2 which does not contain nanotube, the argon atoms covered all of the region of the hole on the graphene sheet. The reason for this result is the $r_{min} = \frac{1}{\pi} \sigma = 1.12\sigma$ range
for the intermolecular Lennard-Jones potential which we defined at chapter 2. Since the argon atoms confined in the nonotube with length about $\sim 50A^0$ in Model-1 and Model-3, the Argon-Carbon interactions according to $\sigma_{\text{Ar-C}}$ which we defined in chapter 2, cannot go beyond this range and they just covered a ring-area of the cross section of the nanotube which makes sense. For the Model-2, we are dealing with a hole and the argon flow after getting through the hole since there is no carbon atom, they can go beyond that range and they covered the whole cross-section area of the nanotube. To demonstrate this phenomenon better we made this results from another point of view.

![Figure 4.15: The top-view of the nanotube in Model-1. The red circles demonstrate the carbon atoms which make single-walled nanotube and green crosses show the argon atoms. Both X and Y positions are in angstrom units.](image)

Figure 4.15: The top-view of the nanotube in Model-1. The red circles demonstrate the carbon atoms which make single-walled nanotube and green crosses show the argon atoms. Both X and Y positions are in angstrom units.
Figure 4.16: The top-view of the hole on the graphene wall in Model-2. The figure (a) shows the graphene wall made by carbon atoms showed by red circles and the argon atoms passing through the hole inside the wall indicated by green crosses. Figure (b) demonstrates the flow area deeply. Both X and Y positions are in angstrom units.
Figure 4.17: The top-view of the nanotube and the hole on the graphene wall in Model-3. The figure (a) shows the graphene wall made by carbon atoms and SWNT are shown by red circles and the argon atoms passing through the SWNT and the hole on the wall are indicated by green crosses. Figure (b) demonstrates the flow area deeply. Both X and Y positions are in angstrom units.

The \( \sigma \) in Lennard-Jones potential has been defined to find at which distance the intermolecular potential is zero. In other words, the \( \sigma \) plays the role of measurements of the distance between two non bonding particles which is so-called Van Der Waals radius and is equal to one-half of the internuclear distance. If we take a look at the figures (2.7) and (2.8), it is obvious that there is a slightly greater than distance of \( \sigma \) \( (r_{\text{min}} = 1.12\sigma) \), therefore potential energy between two particles reaches a minimum value which indicates a zero force as we have shown in the figure (2.8). In fact, we are representing the most stable region for the pair of particles to remain in that vicinity once an external force is applied [24]. By introducing this fact, now we could explain why for the model which does not have SWNT, the argon atoms have covered all of the hole region which is empty of carbon atoms. Since, in the other models we have a SWNT with a length of \( \sim 50A^0 \), the argon and carbon atoms interact with each other continuously along the length of the nanotube with respect to \( \sigma_{\text{Ar-C}} \) we previously defined previously. So, the argon atoms were going to take a determined orientation with respect to the most stable situation defining by the \( \sigma_{\text{Ar-C}} \) from the SWNT. That is why in Model-1 and Model-3 the argon atoms have taken positions like a ring since they have chosen the minimum energy position.
with respect to the nanotube. For the Model-2, this argon-carbon interactions just happened between the perimeter carbon atoms on the graphene wall, so the argon atoms have this chance to cover all of the region, and when we added a nanotube to Model-2 to have Model-3, we have seen that the pattern is the same for Model-1 which confirms that the effect of carbon nanotube is much larger than the effect of graphene hole on fluid flow positions. We will see that if we go a little more than the length of nanotube, the pattern would be sort of combinations of Model-1 and Model-2 which will lead us to the carbon composites having liner treatments. If the argon-carbon interaction constantly continued, the argon atoms have an inclination to take the previous orientation for the most stable position which the force is zero.

The other aspect we tried to investigate is how the flow atoms go through the confinements of the models from the side view of the models such as X-Z or Y-Z projections. To meet deeply this phenomenon, the argon atoms just inside an imaginary cylinder with radius $\sim 8A^0 - 10A^0$ and length $\sim 10A^0 - 20A^0$ about the mouth of the real SWNT or graphene wall of the models which is the origin of this imaginary cylinder have been considered. It decreases the overlapping of argon atoms and helps us to see how they pass through the nanotube.
Figure 4.18: Y-Z trajectory of the Model-1. The figure (a) demonstrates the argon atoms inside an imaginary cylinder with radius $\sim 10\text{Å}$ and length $\sim 20\text{Å}$. Moreover, figure (b) shows the argon flow inside an imaginary cylinder with radius $\sim 8\text{Å}$ and length $\sim 10\text{Å}$. The red plus signs demonstrate the single-walled carbon nanotube, and the green cross signs show the argon atoms. Both measurements are in angstrom units.
Figure 4.19: Y-Z trajectory of the Model-2. The figure demonstrates the argon atoms inside an imaginary cylinder with radius $\sim 10\,\text{Å}$ and length $\sim 10\,\text{Å}$. The red circles demonstrate the rigid graphene wall with a hole and the green cross signs show the argon atoms. Both measurements are in angstrom units.

Figure 4.20: Y-Z trajectory of the Model-3. The figure (a) demonstrates the whole view of the model with argon atoms inside an imaginary cylinder with radius $\sim 8\,\text{Å}$ and length $\sim 20\,\text{Å}$. In figure (b) to show deeper point of view of figure (a) we just considered the region we have the argon atoms. The red circles demonstrate the single-walled carbon nanotube and the graphene sheet, and the green cross signs show the argon atoms. Both measurements are in angstrom units.

According to the figures which demonstrate the Y-Z trajectories of argon atoms, it is clear that the argon flow when they neared to the mouth of the confinements (SWNT or graphene hole), they got narrower to pass through the confinements. The figure (4.18.a) which depicts how the argon flow inside the imaginary cylinder with radius $\sim 10\,\text{Å}$ and length $\sim 20\,\text{Å}$ treats when reaches the nanotube. They were going to arrange a narrower bulk which looks like a ring as we have shown it
in figure (4.15). In the figure (4.18.b), as we decreased the imaginary cylinder scales with radius \( \sim 8A^0 \) and length \( \sim 10A^0 \), we will see the number of atoms outside the ring like pattern which the argon atoms inclined to make decreases. In fact, what plays here an important role is the effect of the carbon atoms near the mouth of the nanotube. Since the argon flow go far away from the mouth of the nanotube, the inclination to be stable in a ring like pattern decreases and the argon flow goes to cover all of the cross section of the nanotube and the final pattern will look like the pattern for Model-2 except the middle ring which that does not have. The figure (4.19) demonstrates that the argon flow of Model-2 passing through the hole on the rigid graphene sheet got narrower as they got closer. This pattern continues after the hole symmetrically too. We used an imaginary cylinder with radius \( \sim 10A^0 \) and length \( \sim 10A^0 \) for the argon flow. As the flow bulk got closer to the hole, they took a pattern like cylinder with radius \( \sim 6A^0 \) the same the radius of the hole on the graphene sheet and length \( \sim 2A^0 \). In other words, \( \pm 1A^0 \) about the hole position, the argon flow wants to take the most stable position which the force comes from the LJ potential is zero. The most interesting point is why the argon flow covers the whole cross section area about the mouth of the hole where in Model-1 the argon flow made a ring pattern. Moreover, for Model-3 too the flow got narrower to pass through the hole attached to the nanotube. In the figure (4.20) an imaginary cylinder with radius \( \sim 8A^0 \) and length \( \sim 20A^0 \) has been employed. This method helps us to consider the argon atoms in the aforementioned region for investigating more deeply. In the figure (4.20.b) we can see the effect of the graphene nanostructures easily which changed the
initial pattern of the argon bulk and they have been kept at that condition because of the presence of the nanotube. To apprehend this phenomenon explicitly we bring on figure (4.21).

![Figure 4.21: Y-Z trajectory of the Model-3.](image)

In fact, we have increased the radius of the imaginary cylinder which the argon atoms are supposed to be inside of it for $\sim 2A^0$ and we kept the length the same before at $\sim 20A^0$. That’s why we have some argon atoms offside the tubular pattern. By changing the radius we still have the same condition likewise figure (4.20) $\pm 1.5A^0$ about the graphene sheet. We can explain this phenomenon as when the argon atoms reached the graphene sheet, in fact the perimeter carbon atoms
around the hole play a role like they put a multi-walled carbon nanotube with length 1 carbon atom, however these atoms just played a role like MWNT and they are not. That’s why the argon atoms could take the whole cross section area in comparison to SWNT which ring pattern occurred. To clear it out we can picture the X-Y point of view of figure (4.21).

![Figure 4.22: X-Y trajectory of the Model-3. The figure demonstrates the cross section view of the model with argon atoms inside an imaginary cylinder with radius $\sim 10A^0$ and length $\sim 20A^0$. The red circles demonstrate the single-walled carbon nanotube and the graphene sheet, and the green cross signs show the argon atoms. Both measurements are in angstrom unit.](image)

As we have seen we have some off-ring argon atoms, since we demonstrated the top view of the model. Thus, the atoms from the bulk inside the imaginary cylinder can be shown in this graph too. In addition to this, we did have some atoms
outside of the nanotube because we have considered atoms in radius \( \sim 10A^0 \) where the hole radius is just \( \sim 6A^0 \).

To clear out why the argon flow has been gotten narrower near the confinements such as, nanotube and graphene wall, vector plots of the argon flow have been demonstrated. Each vector is related to an argon atom and the starting point of the vector is the coordinates of the argon atom. The direction of the arrow has been calculated using the angle of the velocities in this plane: \( \alpha = Arctan\left(\frac{V_y}{V_z}\right) \), and the length of the vector means the speed of the atom in this plane: \( V = \sqrt{V_y^2 + V_z^2} \). In addition, we have considered that the Tangent is a \( \pi \) radians periodic function.

Figure 4.23: Vector plot of the argon flow passing through Model-1. The dashed box has shown the side-view of the SWNT, and the blue arrows demonstrated the direction and speed of the movements of the argon flow through SWNT in Y-Z plane. Both measurements are in angstrom units.
Figure 4.24: Vector plot of the argon flow passing through Model-2. The dashed box has shown the side-view of the graphene wall, and the blue arrows demonstrated the direction and speed of the movements of the argon flow through SWNT in Y-Z plane. Both measurements are in angstrom units.
Figure 4.25: Vector plot of the argon flow passing through Model-3. The dashed box has shown the side-view of the SWNT and graphene wall, and the blue arrows demonstrated the direction and speed of the movements of the argon flow through SWNT in Y-Z plane. Both measurements are in angstrom units.

Performing these graphs lead us to the point that the argon flow tried to pass through the confinements. That’s why we had some empty areas in figures near the confinements. In other words, the argon flow has been sucked into the confinement through the push of the moving graphene wall. Due to the length of the arrows inside the nanotube we could say that the argon flow kept its velocity inside the confinement too.

The development of the mean position and velocity of the argon atoms in each time steps has been investigated too.
Figure 4.26: The average X-direction of the argon atoms in each time steps. The red lines point demonstrates Model-1, the green one Model-2, and the blue lines point shows the mean value of the X-direction for Model-3. The position measurements are in angstrom unit.

According to the figures (4.23) and (4.24) which demonstrated the mean positions in X and Y direction for argon flow over time steps, the X values fluctuate about $27.5\text{Å} - 29\text{Å}$, and Y values fluctuate about $27.5\text{Å} - 29.4\text{Å}$. We can explain the reason of this phenomenon by returning to the chapter 2 when we defined our three models. If we remember, all of our models contain a confinement like SWNT and graphene wall with a hole which these confinements have a circular cross section.

Figure 4.27: The average Y-direction of the argon atoms in each time steps. The red lines point demonstrates Model-1, the green one Model-2, and the blue lines point shows the mean value of the Y-direction for Model-3. The position measurements are in angstrom unit.
The origin of this confinements is $X = 27.13A^0, Y = 26.26A^0$. Thus, the average positions of the argon atoms are around the origin of the confinements, it means the number density of the argon atoms around the confinements is much larger than the number density of the argon atoms outside of the confinement. In other words, by employing the moving graphene wall we succeed to send the argon atoms inside the nanotubes.

Figure 4.28: The average Z-direction of the argon atoms in each time steps. The red linespoint demonstrates Model-1, the green one Model-2, and the blue linespoint shows the mean value of the Z-direction for Model-3. The position measurements are in angstrom unit.
4.4 The effect of moving graphene wall

In our simulation we set the velocity of the graphene wall to $\left( \frac{0.05 \text{Å}}{1000 \text{timestep}} \sim 18 \frac{\text{Å}}{\mu s} \right)$. Hereby, to find the effect of the moving graphene wall we decided to move the graphene wall towards the nanotube faster and consider the effect of this change in pressure with respect to previous calculations. Thus, we changed the velocity to $\left( \frac{0.1 \text{Å}}{1000 \text{timestep}} \sim 36 \frac{\text{Å}}{\mu s} \right)$ which is the double value of the previous velocity and repeat all of the previous calculations for 600000 MD time steps, then divided up the time steps into six blocks, and found the standard deviation and its error in each block. Hence, we provide all of the results with the figures below.
Likewise the previous results, we kept the temperature constant using the re-scaling the velocity and let the energy fluctuate since we are dealing with the NVT ensemble.

Figure 4.30: Temperature in reduced units versus MD time steps. The red line demonstrates the development of the temperature over time for Model-1, the green line for Model-2 and the blue one for the Model-3.
Figure 4.31: The development of the average energy per volume over time for argon fluid through different models. The red solid line demonstrates the average energy and violet lines point shows its error for Model-1, the green solid line shows the average energy and the sky blue lines point pictures its error for Model-2, and the blue solid line pictures the energy and yellow lines point shows its error for the Model-3. All of the energy measurements are in reduced units.

The energy in figure (4.28) in which we doubled the velocity of the moving graphene wall in comparison to figure (4.2) has increased surprisingly. Since, we run the second code just for 600000 MD time steps, the system does not reach the thermal equilibrium, but obviously we can see the trend of the changing of the energy for the different models. By comparing the numbers, we can conclude that when we increased the velocity of moving wall, in fact, we have increased the number of interactions. Since, in the figure (4.2) we have numbers between $-0.1$ and $0.1$ for the reduced energy. On the other hand, in figure (4.28), we have numbers between $0$
and $-2500$. When we put the amount of the potential energy and the kinetic energy under individual consideration, we see what affects the total energy is the share of the potential energy by the Lennard-Jones potential. It means, when we increased the velocity of the moving wall, the share of the potential energy is larger than the share of the kinetic energy. That’s why all of the total energy for the second case is in the negative part of the energy. Nevertheless, in the first case, the share of the potential energy and the kinetic energy are close to each other.

Figure 4.32: The development of the average pressure of the nanotube over time for argon fluid through different models. The red lines point demonstrates the average pressure for Model-1, the green lines point shows the average pressure for Model-2, and the blue ones pictures for the Model-3. All of the pressure measurements are in reduced units.
Figure 4.33: The comparison of average pressure of the nanotube for the models with using different velocity for moving graphene wall. The three red, green, and blue solid lines represent the changing of the average pressure of the nanotube over MD time steps for Model-1, Model-2, and Model-3 respectively. In addition, the three violet, cyan, and yellow lines represent the development of the average pressure of the nanotube versus MD time steps for Model-1, Model-2, and Model-3. All of the measurements are in reduced units.

When we compare these two sets of figures, we could find out that for the sets which we increased the velocity of the moving graphene wall, we have a shift to the origin of time for the pressure, but the approach of the trends is the same. It means, e.g. for Model-3 about 450000 MD time steps the pressure is maximum, we have this maximum for the case we changed the velocity (Model-3 2x) about 350000 MD time steps and so on. In other words, increasing the velocity of the moving graphene wall makes the fluctuations happen sooner.
CHAPTER V

CONCLUSIONS

In this study, three different models contain single-walled carbon nanotube armchair (10,10) (Model-1), a rigid graphene sheet with a hole on it (Model-2), and a combination of both (Model-3) have been employed to investigate the physical treatment of the liquid argon passing through these models using a moving graphene wall as device to push the argon flow towards the confines of the system instead of bombarding the argon atom like bullets. For the interactions between argon and carbon atoms, the 12-6 Lennard-Jones potential and a mechanical set of variables to simulate our models using molecular dynamics (MD) has been defined. Using a re-scaling velocity algorithm we kept temperature at a constant value to have NVT ensemble to start consideration the models. Since the fraction of the collision of the atoms with each other with respect to the total collision dominates the collision with the walls, it is common to use the periodic boundary conditions. In addition to this, due to the size of our models which is large enough ∼ 5000 atoms, during the MD time steps we have found out that the total energy is about a constant value which has assured us we have reached a thermodynamical equilibrium which is a good point in our simulations. Then the pressure of the flow passing through the models has been investigated. We have observed the pressure of the argon flow in Model-1 is larger than Model-2 and
Model-3. In other words, when we have used the graphene sheet as a confinement, the pressure decreased in comparison to the model which we have used SWNT as a confinement. Thus, in Model-3 which we have the combination of them, we did have similar pressure like we had for Model-2. We also tried to investigate at which position along the nanotube axis, the pressure starts fluctuating. We have reported about $80A^0 - 120A^0$ where the moving graphene wall covered, the pressure fluctuates a lot and in some parts we did have a bunch of errors. Then in interval $50A^0 - 80A^0$ the pressure fluctuations start getting narrower since the argon flow has been blocked by the moving graphene wall which stopped at $\sim 80A^0$ and the confinement at $\sim 50A^0$. Then in $0 - 50A^0$ just the flow pressure inside the confinement has been considered. We have shown that the pressure inside the SWNT (Model-1) is much larger than the other models. The rate of changing the velocity of the flow inside and outside of the confinements used in our models has been reported too. With no doubt, the fluid flow starts getting slower when reached the mouth of the SWNT or the hole on the graphene sheet. In addition to this, we have seen when the argon flow reached the rigid graphene sheet, its velocity dropped dramatically and then starts increasing to get closer to a constant value. In addition to velocity alongside the nanotube axis ($V_z - Z$), an analysis about the radial speed has been performed too. We have calculated the radial speed $V_r = \sqrt{V_x^2 + V_y^2}$ versus the radius of the nanotube or hole on the graphene sheet $\sim 6A^0$. We have apprehended the argon atoms passing through the confinement contains SWNT, and inclined to take some ring patterns. On the contrary, in Model-2 which we had just a graphene wall as a confinement, the argon
atoms have covered all of the cross-section area of the hole. Moreover, using the side view of the trajectories, we have seen the argon atoms start getting narrower to pass through the confinements and made an empty area $\pm 2A^0$ about the mouth of the confinements. We have tried to explain the reason of this phenomenon by observing the vector plots of the velocities of the argon flow which have shown us they have been sucked into the confinement about this area. For the last thing, we have repeated the simulations with a different velocity for the moving graphene wall to apprehend how this affects our results. We did show this made a shift in our results and all of the occurrence in the system would happen sooner because the argon flow has moved faster. Unfortunately, we did not reach the thermodynamical equilibrium anymore likewise previous simulations. To wrap it up, the fluid flow in carbon nanotubes are dramatically related to the unconfined fluids.

For the future work, we could perform simulations using multi-walled carbon nanotubes (MWNT), or instead of armchair (n,n) we can use zigzag (n,m) in our models. Moreover, we can change the fluid in our models. One of the most promising fluid and hard to model is water. The water-water interaction, due to the hydrogen-bond network is usually modeled by TIP4P rigid body potential, and the carbon-water interaction can also define by Lennard-Jones potential like our models [25]. These simulations and amazing fluid conduction of carbon nanotubes lead us to investigate applications of these models in drug delivery in living cells. We do expect to use carbon nanotubes as nanofluidic devices such as, sensors, filters, actuators, reactors, and channels [26].
BIBLIOGRAPHY


[5] Reynolds, Osborne; An experimental investigation of the circumstances which determine whether the motion of water shall be direct or sinuous, and of the law of resistance in parallel channels. Philosophical Transactions of the Royal Society 174 (0): 935–982. (1883)


