1 INTRODUCTION

1.1 Motivation and statement of problem

According to United Nations Panel, emissions of greenhouse gases were causing in
global warming up to 5.8 °C over the next 100 years if it not overcome yet (IPCC,
2001). Carbon dioxide (CO₂) is the one of greenhouse gas and it emission will cause the
climate change. Climate change refers to a change of climate that is attributed directly
or indirectly from the human activity that could affects the composition of the global
atmosphere (IEA, 2010). According to IPCC(2001) it is almost certain that emissions of
greenhouse gases will result in the planet becoming warmer, disappearing glaciers, loss
of biodiversity and rising sea levels. This is supported by the Arctic Climate Impact

Figure 1-1 show CO₂ from the fossil fuel is the primary contributor in greenhouse gas
that produces from the human activities compare with other source of gas. This trend
will continue to grow until 40.2 Gigaton (Gt) by 2030 (IEA, 2010). Therefore, CO₂
capture and storage (CCS) is the best of approach to reduce CO₂ emission and it is
considered as a critical technology for reducing atmospheric emissions of CO₂ (Folger,
2013). CCS is consisting with three step processes which are including CO₂ capture,
transportation of CO₂ and geological storage or sequestration (Li et al., 2011). Generally, there are three effective options for CO₂ capture such as pre combustion
process, oxy fuel combustion and post combustion (Drager et al., 2012)

Figure 1-1: Different greenhouse gases in total global emissions in 2004
(Source: IPCC, 2007)
The increasing emissions of CO₂ were already believed to be affecting the climate change (IEA, 2012). In order to reducing this problem, there are many technologies that available for separation and capture CO₂ from gas streams, although they have not been designed for power plant scale operations. These technologies were based on different physical and chemical processes such as chemical and physical absorption, adsorption, membrane separation and other biological absorption (Kohl and Nielsen, 1997). The choice of a suitable technology depends on the characteristics of the flue gas stream, which is depend mainly on the power plant technology (Rao and Rubin, 2002).

In this study, the computer simulation technique applied was the molecular dynamics (MD) simulation. According to Maginn and Elliott (2010), MD is a powerful tool to help comprehend and reveal intermolecular interaction behaviour between the solute and the solvent molecules during the carbon capture process. The solute and solvent used in this study are CO₂ and 1, 6 Hexamethylenediamine, HMDA + water, H₂O. It also the best approach chosen to study and enhances the molecular distribution of the system inside the absorption solution (Farmahini, 2010). The concept of Newton’s second law will be used to simulate the dynamic aspect of the system. In addition, the coordinate system will be used to calculate the radial distribution function (RDF), and self diffusion coefficient which could be used to describe the molecular interaction behaviour during CO₂ captures (Adam et al., 2014).

1.2 Objectives

The objective in this research is:

- To study the effect of the temperatures on intermolecular interaction of 1, 6-Hexamethylenediamine (HMDA) and CO₂ in absorption process by using molecular dynamic (MD) simulation technique.

1.3 Scope of this research

The scopes of this research are:

- Radial distribution function (RDF) is used to study the intermolecular interaction for tertiary system (HMDA + water + CO₂) by using MD simulation at temperature 313K and 333K.
• The optimum molecular interaction will be determined by observing the highest intermolecular interaction between molecular while simulating the absorption process at different temperature.
• Mean square displacement (MSD) is used to determine the self diffusion coefficient of HMDA and CO₂ inside the simulation system at temperature 313K and 333K.

1.4 Main contribution of this work
The increasing emissions of CO₂ got higher attention by all peoples in this world. Due to this challenge, many researches and investigations have been made by experimental or simulation to find the efficient solution to solve this problem. In this research, the best option to reduce the emission of CO₂ is by capture CO₂ before it release to the atmosphere. The common process to capture CO₂ in industries is by using amine based absorption in post combustion process. The typical solvents used to absorb CO₂ are Monoethanolamine (MEA), Methydiaethanolamine (MDEA) and etc. However, the solvent that commonly used also have the disadvantages in terms of corrosion, cost and properties. The purpose of this thesis is to provide the information in term simulation data for the new solvent which is HMDA. The selection of HMDA solvent in this study due to its ability is comparable with MEA solvents and has the potential to be used as new solvent for carbon capture (Singh, 2011).

1.5 Organisation of this thesis
The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provide a description of sequences in carbon capture process (CCS). It sequences was started from CO₂ produced from fossil fuels burning until storage option. A general description has been made inside this chapter about gas purification process and amine based absorption. Besides that, this thesis also provides the detail explanation in MD simulation in term of forcefield, interactions consist in the simulation and ensembles.

Chapter 3 give the review the general description about the material studio software that was used. Besides that, this chapter also provide the explanation in methodology to perform the MD simulation from start until analysis of the result simulation.