Intermolecular Interaction of Monoethanolamine, Diethanolamine, Methyl diethanolamine, 2-Amino-2-methyl-1-propanol and Piperazine Amines in Absorption Process to Capture CO_2 using Molecular Dynamic Simulation Approach

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Abstract—Many active researches struggle to identify a solution towards problem of effect excessive CO_2 emission in atmosphere. Global warming effect happen when there has excess of CO_2 percentage in atmosphere. Amine-based absorption process technology is selected in this work because their efficiency to capture CO_2 up to 90%. The aim of this paper is to study intermolecular interaction of MEA, DEA, MDEA, AMP and PZ amines based absorption process to capture CO_2 using molecular dynamic (MD) simulation. MD simulation was run under condition 313K and 1 atm. It used NVE ensemble at 200ps and NVT ensemble at 1ns. The results were interpreted in term of intermolecular interaction by using Radial Distribution Function (RDF) analysis. It was found that AMP solvent shows the highest tendency to make intermolecular interaction with H_2O and CO_2 compared to MEA, DEA, MDEA and PZ. MDEA has the weakest intermolecular interaction with CO_2 among

others. Thus it is required that MDEA to blend with promoter or other amine for enhance the reaction with CO_2. The blend of conventional amine i.e. MEA, DEA and MDEA with activator amine is expecting to increase CO_2 absorption capacity and reduce heat regeneration requirement.

Keywords— Absorption Process; Carbon Dioxide Capture; Alkanolamine; Activator Amine; Molecular Dynamic Simulation

1. INTRODUCTION

It is well known that carbon dioxide, CO_2 emission will cause many disadvantage especially towards our environment and human health. Up to 90% emission of CO_2 is from burning of fossil fuels [1]. The average annual rate of CO_2 emission is increasing between 2000 and 2014 (2.3%) and expectedly will be rapid rise in next another year. Due to high levels of CO_2 concentration, there has many Protection Act enacted to give public consciousness towards our environment. In Malaysia, there has Department of Environment which is under of Ministry of Natural Resources and Environment (NRE). Goals to be achieved by Department of Environment are emission reduction of greenhouse gases (GHG), strengthen environment quality act (1974), protecting ozone layer and enhance awareness on environment and climate change. From this, it can be seen that government especially, Malaysia are very concern about environment and CO_2 emission problem. To support effort by government, many researches have done to find the best technology to capture CO_2 acid gases.

The techniques option for CO_2 separation and capture available currently are absorption, adsorption, cryogenics, membranes and microbial or algal systems. In this research, absorption process using amine solvent solutions was selected according to their advantages such as most applicable for CO_2 [2], fast reaction at low partial pressure of CO_2 [3] and suitable for retrofitting absorption process power plant [4]. The exothermic heat of reaction involved in absorption process between amine solvent and CO_2 is reversible reaction. There are many types of amine extensively applied and studied in CO_2 absorption process but in this study monoethanolamine (MEA), diethanolamine (DEA), methy diethanolamine (MDEA), piperazine (PZ) and 2-amino-2-methyl-1-propanol (AMP) were selected. The selection of amine is based on its class of solvent alkanolamine such as primary, secondary, tertiary, cyclic and sterical amines. The selection of amine solvent is important because it will influence the capacity CO_2 capture, the CO_2-amine reaction rate, amount of energy consumption in operation of the process, viscosity and corrosiveness [5], [6]. In this research, more attention takes into account is the properties of amines itself because different types of amine will have different reaction mechanism with CO_2 gas. The interaction between chemical solvent as basicity and CO_2 as acidity produce a reversible acid-based reaction in absorber column. The reaction of CO_2 and amine will produce different compound such as carbamate, bicarbonate and carbonate ion. These chemical products will influence the CO_2 absorption process. However, the challenges of amine-based absorbent for CO_2 absorption process are high energy demand for regeneration part, limited CO_2 absorption capacity, degradation and corrosion [7]. The aim of case study is to know which amine can show fast intermolecular interaction with CO_2 and water and discover causes for it happened. The ion molecules form has own stability which effected to stripping process later.

There are many reported literature related to various amine-based absorbents tested for CO_2 absorption process. Primary and secondary amines such as MEA and DEA, respectively will form a carbamate ion when react with CO_2. Tertiary amine such as MDEA and TEA which will form bicarbonate ion by hydrolysis process because it cannot form carbamate ion due to lack hydrogen atom attach at nitrogen atom. According to Choi et al. (2012), the reaction rate of CO_2 absorption process by using TEA is lower compared to MEA and DEA [8]. Nuclear magnetic resonance (NMR) spectroscopy was used in this research. It was reported that hydroxyl group in MEA and DEA attract electron density from other atoms to make molecular electronic distribution. Other than primary, secondary and tertiary amines, additive amine such as AMP and PZ also gain attention in application of CO_2 absorption process. Chakraborty et al. (1988) studied molecular orbital approach to substituent effects in amine-CO_2 interactions. The substituent mentioned was methyl and alcohol groups. From this research, it shows that steric hindered amine (where methyl substitution at the α-carbon atom in primary or secondary amine) will influence the reactivity and selectivity in amine-CO_2 reactions [9]. As pointed out by Hook (1997), CO_2 absorption capacity by using steric hindered amine was compared with MEA amine. In this research mentioned, increase substituent at the α-carbon atom will cause reduce absorption rate [10]. Stability of carbamate ion produce by steric hindered amine is reduced and it will directly shift to bicarbonate ion through hydrolysis. Moreover, sterically hindered amine require less heat for regeneration compare with MEA [7]. Damartzis et al. (2015) proposed optimized process flowsheet design for various amine-based solvents in post-combustion CO_2 capture plants [6]. AMP solvent can enrich the CO_2 absorption and minimize thermal use in regeneration step cause reductions to cost of process. Seo and Hong (2000) studied the effect of PZ on the kinetics of CO_2 with aqueous solutions of AMP. PZ is cyclic secondary diamine. AMP is primary sterically hindered amine. From this study, additional of PZ make reaction rate of AMP aqueous solution with CO_2 to increased [11]. When concentration of PZ increased, the reaction coefficient for AMP mixture will be increased.

In the present study, potential of individual amines i.e. MEA, DEA, MDEA, AMP and PZ in CO_2 absorption process on molecular level will be discussed. The intermolecular interaction analysis using molecular dynamic (MD) simulation will be used in this

study. Many researched doing experiment works to study the CO_2 absorption process using amine solvent are published in open literature. However, this research applied computational tools like MD simulation to study the behaviour of the molecules during absorption process. There have been many advantages using MD simulation in chemistry study. MD simulation approach is used to give more understanding about absorption process in molecular level. By analysing sample using MD simulation, cost of operation can be reduced without purchase chemical substance and expensive equipment [12]. MD simulation also can be used to interpret experimental result and save time consuming when run simulation simultaneously with different computer processor. This computational tools also very powerful when can test sample to predict the thermodynamic properties of sample [13]. Overall, MD simulation appears to be the attractive tools to study absorption process at molecular part. All molecules are evaluated using RDF analysis. This analysis provided in MD simulation and calculation is done by computational method.

Radial distribution function (RDF) is an analysis to see relationship between (*r*), the distance between atom pairs in each of trajectory distance of atom with other neighbour atom and (*g(r)*), the tendency of atom to interact to other atoms. RDF analysis was performed, in which to see intermolecular interaction between atoms of H_2O-CO_2-amine.

This work focus on identification which amine has high intermolecular interaction with water and CO_2 and this interaction will affect the absorption process. MEA, DEA, MDEA, AMP and PZ amines are deciding to be used because it has different physical and chemical characteristic which will influence to their reaction mechanism. All amines are analysed with conditions of 30 wt. %, 313 K and 1 atm. Intermolecular interaction will give insight on how the physical interactions occur between the molecules prior to the reaction. Activator amines such as AMP and PZ are expected to be good potential solvent as it possesses cover the limitation of traditional amine i.e. MEA, DEA and MDEA. Application of activator amines in absorption process is expecting to increase the CO_2 absorption efficiency and reduce thermal energy for regeneration process.

2. THEORY

A. Reaction mechanism for MEA and DEA amines

There are many literatures review the mechanism reaction used conventional solvent amine i.e.; MEA, DEA [14]–[16]. The available literature about mechanism reaction for primary or secondary amine is based on a zwitterion intermediate (one-step carbamate reaction) and two-step carbamate formation. The mechanism reaction for one-step reaction on primary and secondary amine is shown as follows [17] in (1) to (3):

$$2R_1R_2NH + CO_2 \leftrightarrow R_1R_2NH_2^+ + R_1R_2NCOO^- \quad (1)$$

Moreover, the mechanism reaction for two-step reaction on primary and secondary amine is shown as:

$$R_1R_2NH + CO_2 \leftrightarrow R_1R_2NH^+COO^- \quad (2)$$

$$R_1R_2NH^+COO^- + H_2O \leftrightarrow H_3O^+ + R_1R_2NCOO^- \quad (3)$$

The reaction happen in primary and secondary amine is relating with an electron acceptor Lewis acid. A proton on amino group in carbamate ion will be replaced with CO_2 where CO_2 absorption process occurs.

B. Reaction mechanism for MDEA amine

Methy diethanolamine, MDEA is a tertiary amine. The reaction mechanism involve in tertiary amine is not similar as primary and secondary amine. Due to lack of hydrogen atom attach at nitrogen atom make tertiary amine cannot directly react with CO_2 to form carbamate ion. The hydrolysis of CO_2 leading to the formation of carbonic acid. Then, carbonic acid will react with tertiary amine to form bicarbonate ion. The reaction mechanism of tertiary amine with CO_2 can be seen on studies [15], [18]–[20]. The reaction mechanism of tertiary amine, MDEA with CO_2 is show as follows in (4) to (6):

$$CO_2 + H_2O \leftrightarrow H_2CO_3 \quad (4)$$

$$H_2CO_3 + R_3N \leftrightarrow R_3NH^+ + HCO_3^- \quad (5)$$

The overall reaction mechanism is as follows:

$$CO_2 + H_2O + R_3N \leftrightarrow R_3NH^+ + HCO_3^- \quad (6)$$

C. Reaction mechanism for PZ amine

Piperazine (PZ) is a cyclical amine and also a secondary diamine. PZ is same as primary and secondary amine. It will be form carbamate ion, zwitterion ion and protonated carbamate when react with CO_2. The reaction mechanism for PZ solution with CO_2 is show as follows [21] in (7) to (9):

$$CO_2 + 2PZ \leftrightarrow PZCOO^- + PZH^+ \quad (7)$$

$$CO_2 + PZCOO^- + B \leftrightarrow PZ(COO^-)_2 + BH^+ \quad (8)$$

$$CO_2 + PZH^+ + B \leftrightarrow H^+PZCOO^- + BH^+ \quad (9)$$

D. Reaction mechanism for AMP amine

There are a few literature reviews of previous works which discuss the reaction in CO_2-H_2O-AMP system [22], [23]. Since AMP also known as primary amine, it was been adopted the reaction mechanism of primary and secondary amine with CO_2. It also goes through a zwitterion mechanism. AMP has a special characteristic of sterically hindered. Due to steric hindered, carbamate formation from zwitterion easily to dissociated and reduce the resistance of degradation process compared to other alkanolamine. The carbamate ion of AMP-CO_2 is easily to break like tertiary amine, MDEA.

The reaction mechanism for AMP solution with CO_2 is described as follows [24] in (10) to (15):

The overall reaction of CO_2 with AMP solution.

$$\mathrm{CO_2 + RNH_2 + H_2O \leftrightarrow RNH_3^+ + HCO_3^-} \quad (10)$$

Absorption reaction mechanism.

$$\mathrm{CO_2 + RNH_2 \leftrightarrow RNH_2^+COO^-} \quad (11)$$

$$\mathrm{RNH_2^+COO^- + H_2O \leftrightarrow RNHCOO^- + H_3O^+} \quad (12)$$

Regeneration reaction mechanism.

$$\mathrm{RNHCOO^- + H_2O \leftrightarrow CO_2 + RNH_2 + OH^-} \quad (13)$$

$$\mathrm{HCO_3^- \leftrightarrow CO_2 + OH^-} \quad (14)$$

$$\mathrm{CO_3^{2-} + H_2O \leftrightarrow CO_2 + 2OH^-} \quad (15)$$

II. SIMULATION METHODOLOGY

MD simulation was installing in HP240 workstation using software of Material Studio (version 7.0). This software was licensed by Acceryls manufacture. Six steps will perform regarding to simulate the selected molecules as presenting the CO_2 absorption system i.e. molecular structure sketch, geometry optimization, simulation box creation and energy minimization, simulation at equilibrium and production phase, and analysis the last trajectory for output data for RDF in MD analysis. Royal Society of Chemistry database was used to replicate the true behaviour of molecules based on actual absorption process [25]. After replicate the molecular structure of molecules, geometry optimization was run to stabilize the molecular geometry structure under Smart Algorithm and Fine convergence level. Simulation box develop used the amorphous cell calculation, and then simulated for box energy minimization. COMPASS and Ewald models were used for forcefield and summation method calculation, respectively within simulation box [26]. Equilibrium phase under NVE ensemble was run until 200 ps. The aim of long initialization runs was to get a good starting configurations and sample for next production run [27]. Use last frame of sampling from equilibrium phase for further production run. Production phase under NVT ensemble was run until 1 fs. 1 fs time step was used in order to ensure all molecules in simulation box do not overlapping each other [26]. Temperature selected for this analysis was 313 K. Table 1 show the input data for simulation run which based on actual absorption process. The calculation for density mixtures was referred to the Thermodynamic Properties of Chemical and Hydrocarbon" book [28]. All calculation involve in MD simulation for RDF and MSD analysis was refer to manual tutorial provided by Acceryl's Material Studio software [29].

Table 1. Input parameters to analyse the effect different types of amine on the system

Temperature	313 K				
Pressure	1 atm				
Type amines	MEA	DEA	MDEA	AMP	PZ
Density mixture for binary system (g/ml)	1.00088	1.00642	1.00157	0.99366	0.99401
Number of molecule for binary system	A: 50	A: 50	A: 50	A: 50	A: 50
	B: 396	B: 681	B: 772	B: 578	B: 554
Density mixture for tertiary system (g/ml)	0.99244	0.99786	0.99259	0.98399	0.98455
Number of molecule for tertiary system	A: 50	A: 50	A: 50	A: 50	A: 50
	B: 340	B: 580	B: 660	B: 490	B: 478
	C: 23	C: 40	C: 45	C: 34	C: 33

For Radial Distribution Function (RDF) analysis, all the bond involving H, N, O, C atoms were simulated to see the intermolecular interaction between them. Equation (16) was used in the simulator to calculate the RDF values.

$$g_{xy}(r) = \frac{< N_y(r, r + dr)}{\rho_y 4\pi r^2 dr} \tag{16}$$

where, Ny(r, r+ dr) is the number of atom, y in shell of width Δr at distance r, r is the spherical radius, ρy is the density of y atom and x is the reference atom.

III. RESULTS AND DISCUSSION

A. Intermolecular interaction between amine and water for binary (amine+water) and tertiary (amine+water+CO2) systems

Radial distribution function (RDF) analysis is used in this work to study the intermolecular interaction between amines, water and carbon dioxide. RDF data used to plot a graph to study the relationship between the distance of molecules with their neighbouring molecules (*r*) and the tendency of strength interaction between molecules (*g(r)*).

Binary and tertiary system is used to observe the effect of adding CO_2 gas to amine solution. Comparison between intermolecular interactions of amine with water in binary system without CO_2 with in tertiary system with CO_2 is analysed. The strength of amine-water intermolecular interaction which describes dissolving process was discussed in this section. Fig. 1 to 3 show the RDF results of the binary system while Fig. 4 to 6 show illustrates the RDF results of tertiary system for MEA, DEA, MDEA, AMP and PZ solutions.

HO_{amine}: Hydrogen at oxygen in amine; **O_{water}**: Oxygen in water; **N_{amine}**: Nitrogen in amine; **H_{water}**: Hydrogen in water

Refer to Fig. 1 to 6, the peak of interaction will be directed to 1. Peak of interaction approach to 1 due to the system is the ideal gas. After 15Å, it is assuming that the intermolecular interaction between molecules is negligible.

Comparison of binary and tertiary system is discussed based on hydroxyl and amino functional groups. Hydroxyl group in amine was used to increase the solubility in water and amino group leads to reaction with acidic gas [30].

For hydroxyl group, binary system result order is AMP> MDEA> MEA> DEA and tertiary result order is MDEA> AMP> DEA> MEA. The result is read based on the highest to the lowest intermolecular interaction bonded between two selected atoms. PZ amine does not have HO_{amine}-O_{water} interaction because it lack oxygen atom in its molecule structure.

In binary system, AMP (1.75, 2.9029) amine has high tendency to make a bond with water compared to others, the strength percent was about 107% compared MEA. AMP is a primary amine which has steric hindrance. The characteristic of AMP leads to stronger intermolecular interaction with water. AMP is a sterically hindered primary amine but the reaction is similar as tertiary amine [31]. AMP amine is reactive, soluble in water, and easier to regenerate to separate CO_2 gas. It can replace the function of MDEA and compete with MEA and DEA. Tertiary amine with the presence of CO_2 also shows high intermolecular interaction with water.

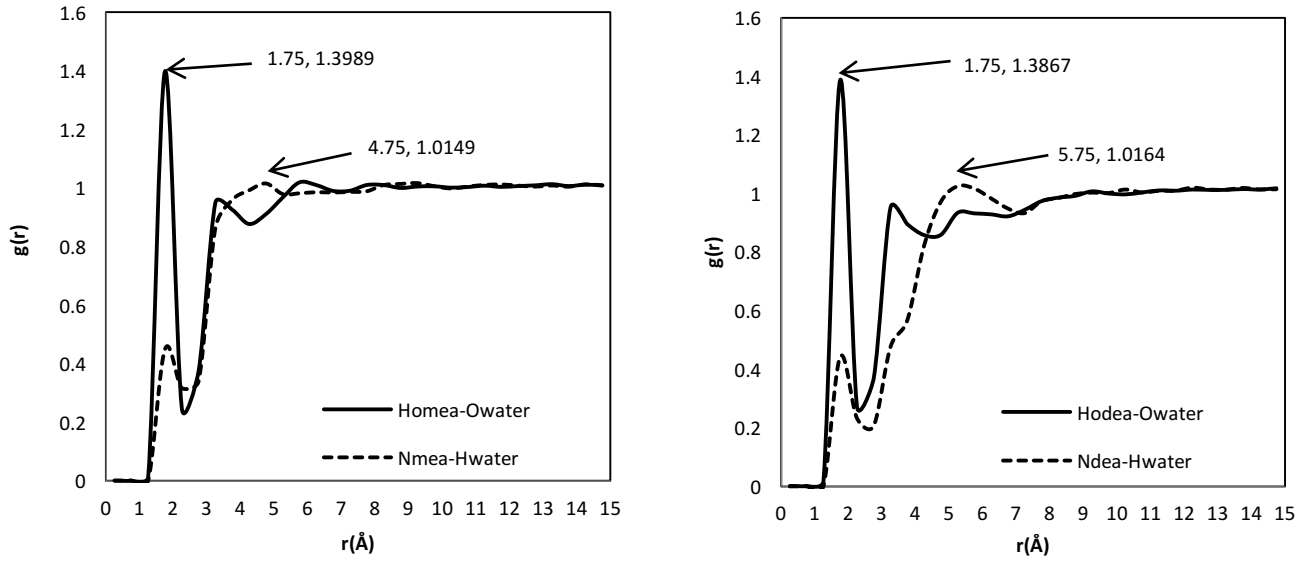


Figure 1: Binary system (a) MEA and (b) DEA solution

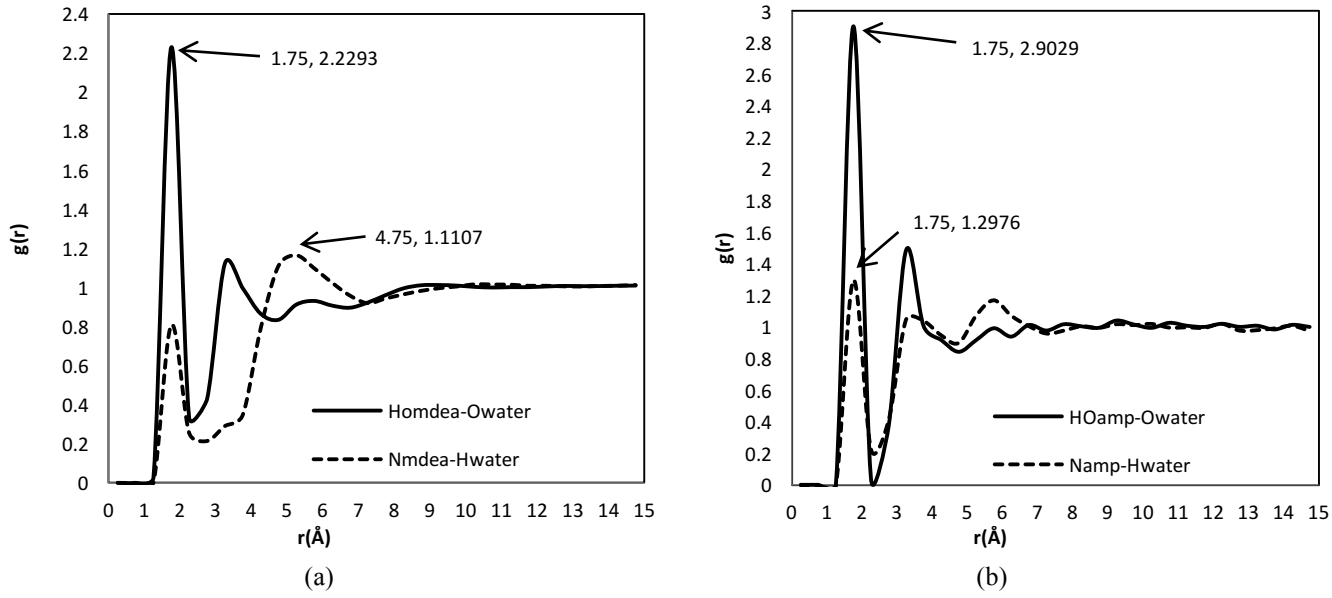


Figure 2: Binary system (a) MDEA (b) AMP solution

In binary system, hydroxyl group of MDEA (1.75, 2.2293) also shows high tendency to make a bond with water similar to AMP. Fig. 7 shows the molecular structure of MDEA. The structure of MDEA can influence the result of RDF. MDEA has two –OH bond which cause it to be more soluble in water compared to MEA and DEA that only has one –OH bond. Besides that, the presence of CO_2 in tertiary system also shows high intermolecular interaction of hydroxyl group in MDEA with water. This is because MDEA cannot directly react with CO_2 to form carbamate ion but has to go through hydrolysis process between CO_2 and water to form bicarbonate ion. The presence of CO_2 and water is essential in order to increase the reactivity of MDEA for CO_2 absorption process.

Based on binary and tertiary system, the intermolecular interaction of DEA with water is in average level. From this finding, it shows that DEA amine as secondary amine has medium potential to dissolve in water and absorb CO_2 in between primary and tertiary amine. Compared to these four amines, DEA has the weakest intermolecular interaction with water. This is because DEA is a secondary amine that is more nucleophilic compared to primary and tertiary amine.

For amino group, binary system result is AMP> MDEA> MEA> PZ> DEA and tertiary result is MDEA> PZ> AMP> DEA> MEA. The highest intermolecular interactions with water for amino group for binary and tertiary system are AMP and MDEA, respectively.

But in the presence of CO_2 in AMP amine solution, intermolecular interaction of amino group with water was decreased about 25.20%. Binary and tertiary result for AMP was (1.75, 1.2976) to (5.75, 1.0364). AMP has α-substitute in molecular structure which led to the reduction of the charge of nitrogen atom [10]. Thus, the interaction of N_{amine}-H_{water} was weaker and it was expected that the reaction rate with CO_2 was slow. The reaction of AMP with CO_2 produce unstable carbamate ion.

PZ showed weak intermolecular interaction in binary system but had strong interaction in tertiary system. PZ amine alone was less reactive for the absorption process. PZ acts as an activator in solvent to accelerate the reaction especially for tertiary amine, MDEA.

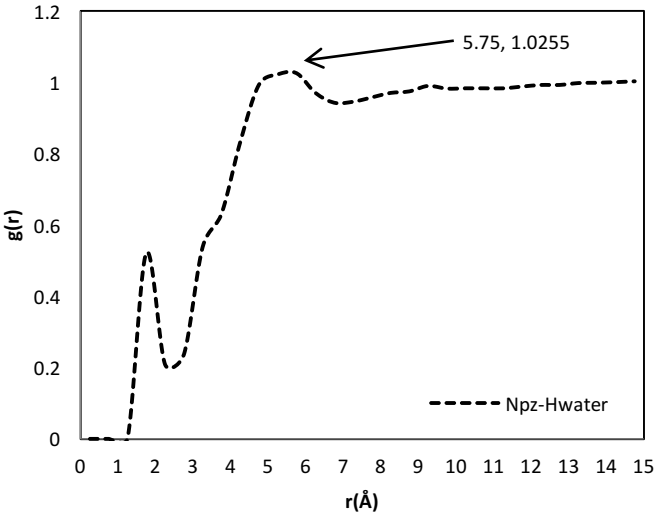
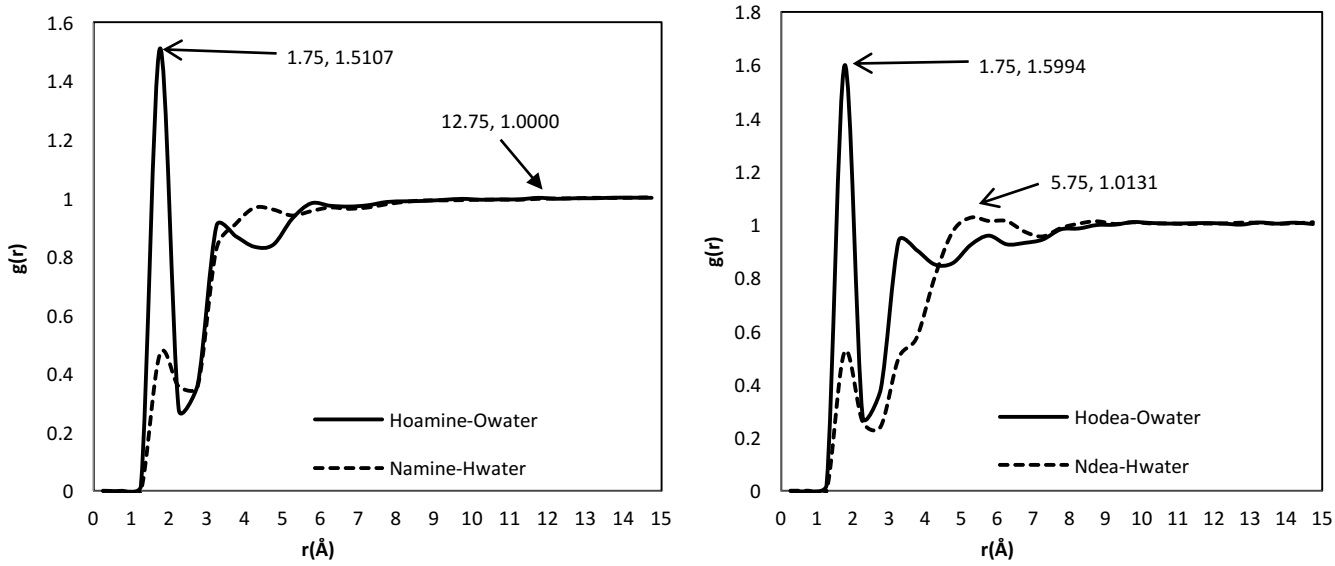


Figure 3: Binary system PZ solution



(a) (b)

Figure 4: Tertiary system (a) MEA (b) DEA solution

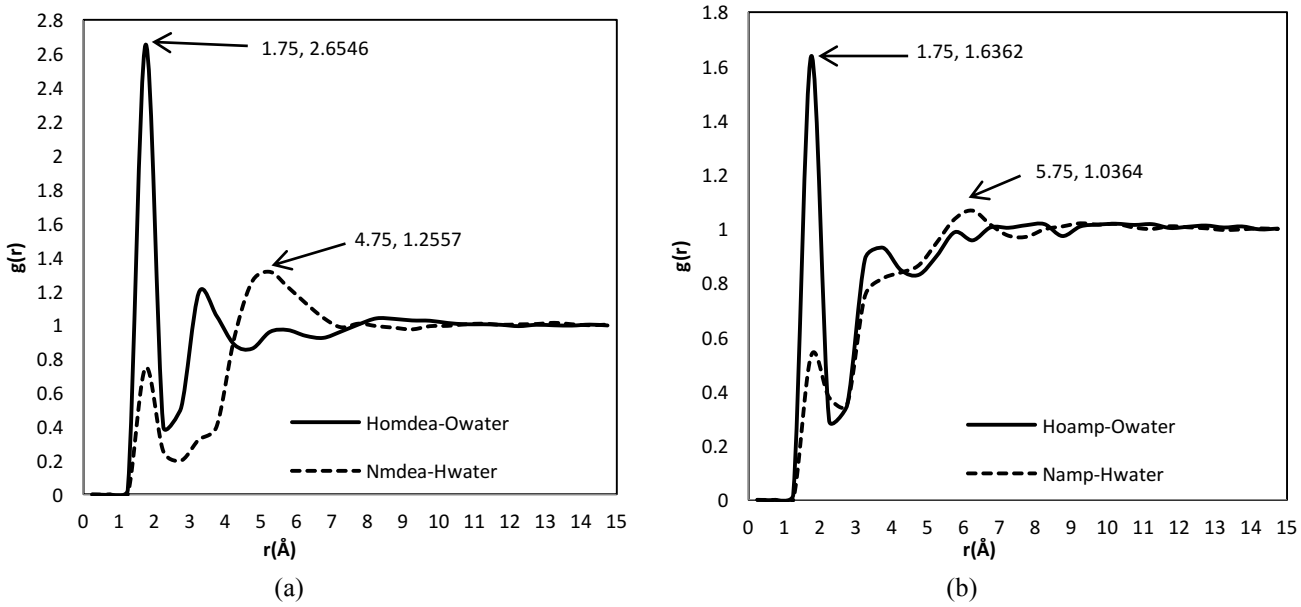


Figure 5: Tertiary system (a) MDEA and (b) AMP solution

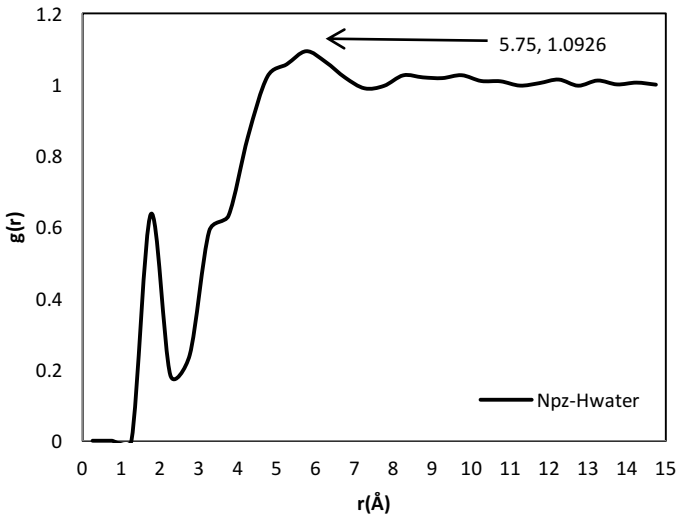


Figure 6: Tertiary system PZ solution

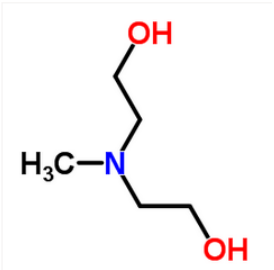


Figure 7: Molecular structure of MDEA

B. Intermolecular interaction between amine solution and CO_2 in tertiary system

The aim of this part is to identify amine solvent that has higher tendency to interact with CO_2. Fig. 8 to 10 show the RDF results of MEA, DEA, MDEA, AMP, and PZ solutions. Same as previous discussion, the intermolecular interaction of amine with CO_2 was determined by comparing which functional group that had more tendencies to interact with CO_2 molecule.

O_{amine}: Oxygen in amine; **C_{co2}**: Carbon in CO_2; **N_{amine}**: Nitrogen in amine

Based on RDF result, the sequence of the highest intermolecular interaction to the lowest for hydroxyl group with CO_2 (O_{amine}-C_{co2}) are MDEA> DEA> MEA> AMP.

At the same distance of r = 3.75 Å, MDEA showed the highest tendency for intermolecular interaction to occur about 8.25% compared to MEA. It is supposed that MDEA has lower intermolecular interaction with CO_2, because it is a tertiary amine. But this intermolecular interaction occurred between hydroxyl groups of MDEA with CO_2. Because MDEA has two –OH bond and other amines only has one –OH bond, molecular structure of MDEA influenced the reaction with CO_2. So this is the reason why RDF results show MDEA was the highest compared others amine.

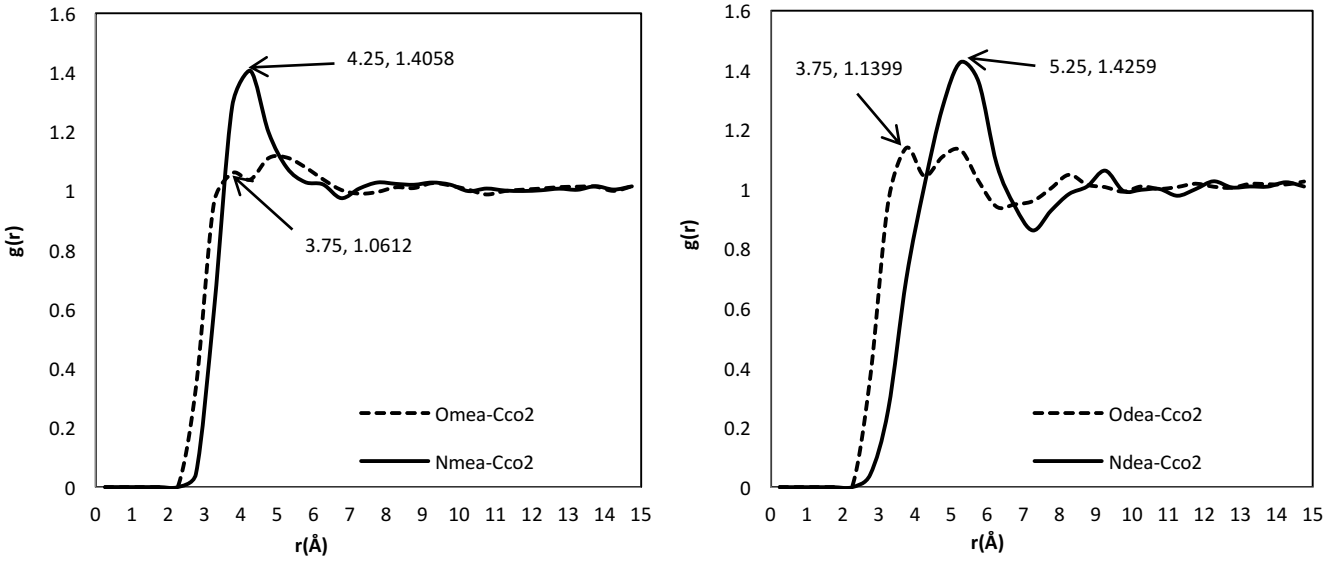
For amino group (N_{amine}-C_{co2}), the trends of the highest interaction to the lowest are MEA> PZ> AMP> MDEA> DEA.

At same distance of r = 4.25 Å, MEA showed the highest tendency for intermolecular interaction to occur about 39.70% compared to AMP. The results obtained have good agreement with the literature study. CO_2 absorption efficiencies reported by Dubois and Thomas (2011) was MEA> PZ> PZEA> AMP> MDEA. MEA was supposed to have the strongest intermolecular interaction with CO_2 because it easily absorbed CO_2 compared to secondary and tertiary amine. Based on Zhang et al. (2008), the trend for absorption performance by experimental were AMP> MEA> DEA> MDEA. Based on this experimental result, MEA and AMP were reactive amine to absorb CO_2. Characteristic of steric hindered amine made AMP to be significant to be used for CO_2 absorption process.

AMP and PZ also showed high value of *g(r)* same as MEA. AMP has sterically hindered amine properties. The reaction mechanism of AMP was proposed by Sartori and Savage (1983) and explained more by Zhang et al. (2008). The reaction of AMP with water produces low stable carbamate ion. Then, carbamate ion reacts with water again through hydrolysis to produce bicarbonate ion and free amine molecule. This free amine molecule will react with CO_2, representing the overall absorption process. However, due to the molecular structure of AMP, the reactivity with CO_2 is lower than MEA [31]. It was reported that when there were more substituents such as methyl and alcohol groups were added, the reactivity of amine towards CO_2 would be decreased. In AMP structure, it has two methyl groups at α-carbon to the nitrogen atom. The presence of substituent methyl group to the amino functional group caused the reaction of AMP with CO_2 to form unstable carbamate ion. Then, the reaction with CO_2 was faster than MDEA [2]. Moreover, the size of molecule will influence the reactivity of amine itself. The molecular weights of MEA and AMP is 61.08 g/mole and 89.14 g/mole, respectively. It shows that AMP size is much bigger than MEA and consequently the intermolecular interaction strength of AMP with CO_2 is lower than MEA even both of amines are categorised as primary amines. Furthermore, the attraction of base (amine) to positively charge CO_2 for zwitterion reaction became slower when the sterically hindered properties were presence [17]. PZ contains two nitrogen atom in its molecular structure which will result to double CO_2 absorption compared to one nitrogen at shorter time interaction. Dubois and Thomas (2011) also stated that activator amine showed good efficiencies for CO_2 absorption. AMP and PZ amines are always chosen to blend with MEA and DEA, because these amines are difficult to separate from amine-CO_2 bond in the stripper. Fig. 11 shows the molecular structure of MEA and AMP.

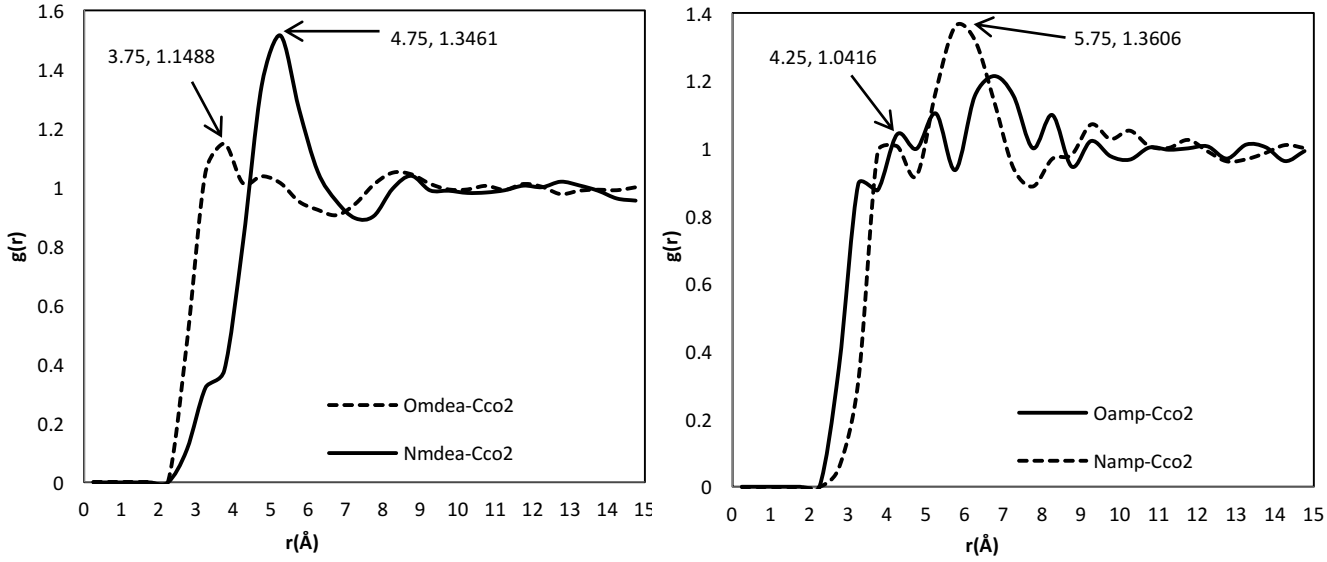
MDEA amine has low tendency to create the intermolecular interaction with CO_2 about 89.47%. This is because MDEA has lack of hydrogen atom attached in amino group there will be no formation of carbamate ion. MDEA cannot directly absorb CO_2. Therefore, it is recommended to blend MDEA with activator amine such as AMP and PZ.

DEA amine also shows low tendency to make intermolecular interaction with CO_2 compared to MEA, AMP, and PZ about 80.95%. DEA is a secondary amine and it is recognised as medium amine in CO_2 absorption efficiency. It was proved that DEA was neither the fastest nor the slowest to dissolve in water and to absorb CO_2. Also DEA poses medium energy requirement for regeneration. In addition, DEA amine gives moderate difficulty to break amine-CO_2 bond.



(a) (b)

Figure 8: Intermolecular interaction of (a) MEA and (b) DEA solutions with CO_2



(a) (b)

Figure 9: Intermolecular interaction of (a) MDEA (b) AMP solutions with CO_2

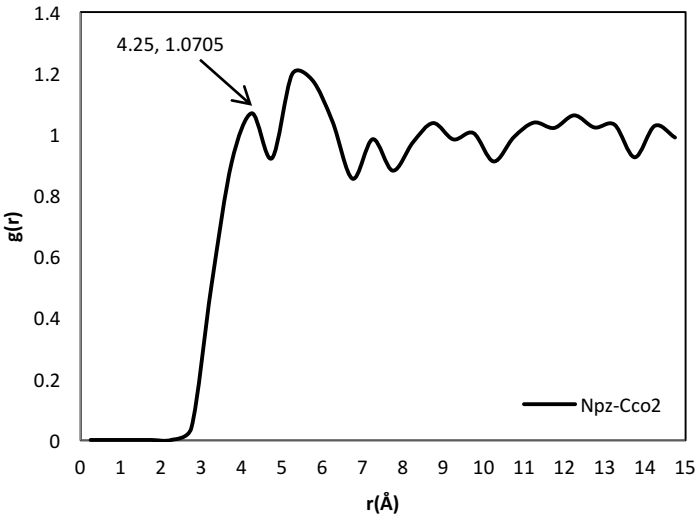
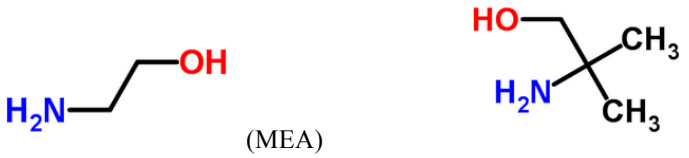


Figure 10: Intermolecular interaction of PZ solutions with CO_2



(MEA) (AMP)

Figure 11: Molecular structure of MEA and AMP

IV. CONCLUSION

The influence of MEA, DEA, MDEA, AMP and PZ in application of CO_2 absorption process through molecular point of view is investigated in this research. The aim of this study is to study the intermolecular interaction of amine-water-CO_2 at molecular level. The hypothesis of this study is when amine molecule has high intermolecular interaction with CO_2, it will enhance absorption process.

From the result obtained, MEA has the highest intermolecular interaction with CO_2. This finding proved MEA is establish known as reactive amine for CO_2 absorption process and be as benchmark solvent for post combustion application process. AMP shows more significant intermolecular interaction with water and CO_2 after MEA. Both MEA and AMP have high reactive toward water and CO_2 but for regeneration process, AMP more significant solvent used. AMP molecular has steric hindered properties which capable to give fast reaction at absorption process and easily separate the CO_2 gas from amine solution at regeneration process. The potential of AMP to become efficient absorbent for absorption and regeneration process is proved from this research. To enhance the efficiency of absorption process and give more CO_2 loading capacity, blended amine with presence of AMP is suggested for next research. Beside AMP, PZ amine also shows high intermolecular interaction towards water and CO_2. The characteristic of AMP and PZ make them be an option to blend with general amine like MEA and MDEA. MDEA amine shows contrary result on intermolecular interaction with CO_2. MDEA is less reactive to be used in CO_2 absorption process since intermolecular interaction of amino group in MDEA with CO_2 was the lowest compared to other amines. The advantage of AMP and PZ in absorption process cause it recommended to be used to blend with MDEA in order to increase MDEA efficiency for CO_2 absorption process.

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