Molecular dynamic simulation of CO_2 absorption into mixed aqueous solutions MDEA/PZ

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Abstract: The mixture of amine absorption process is an approach for mitigation of carbon dioxide (CO_2) from flue gas that produces from power plant. Several experimental and simulation studies have been undertaken to understand this process but the mechanism of CO_2 absorption into the aqueous blended amines such as MDEA/PZ is not well understood and available knowledge within the open literature is limited. The aim of this study is to investigate the intermolecular interaction of the blended MDEA/PZ using Molecular Dynamics (MD) simulation. MD simulation was run under condition 313 K and 1 atm. The thermodynamic ensemble used were 200 ps for NVE and 1 ns for NVT. The periodic boundary is used to visualize the interaction of molecules of the whole system. The simulation method also involved calculation of force field and time integration algorithm.The results were interpreted in terms of Radial Distribution Function (RDF) analysis. It was observed that the hydroxyl group (–OH) of MDEA is more attracted to water molecule compared to amino group (–NH) of MDEA. The intermolecular interaction probability of –OH and –NH group of MDEA with CO_2 in blended MDEA/PZ is higher than using pure MDEA. This finding shows that PZ molecule act as an activator to promote the intermolecular interaction between MDEA and CO_2.Thus, blend of MDEA with PZ is expecting to increase the absorption rate of CO_2 and reduce the heat regeneration requirement.

Keywords: Molecular dynamic simulation; Radial distribution function; Blended MDEA/PZ; CO_2 capture.

Introduction

Carbon dioxide (CO_2) emissions reduction from combustion fossil fuel power plants is a key aspect in the stabilization of global climate change. Post-combustion CO_2 capture from fossil fuel power plants using amine-based solvents such as monoethanolamine (MEA) and methyldiethanolamine (MDEA) is one of the most promising technologies for the abatement of CO_2 gas. Monoethanolamine (MEA) or diethanolamine (DEA) has been proposed by several researchers [1], [2], [3]. Aqueous solutions of monoethanolamine (MEA), a primary alkanolamine, have been extensively studied due to fast reaction rate, low solvent cost and ease of reclamation. But there are some disadvantages of using MEA solution which cause high heat of absorption due to formation of stable carbamate leading to high energy consumption for solvent regeneration in the stripper. Other amines have also been suggested for this application such as 2-amino-2-methyl-1-propanol (AMP) [4], diglycolamine (DGA), and piperazine (PZ) [5], [6], [7]. Sartori et al.[8] proposed the use of sterically hindered amines, because of their high absorption capacity and high absorption rate. Tertiary alkanolamine such as MDEA has a low reactivity with respect to CO_2, due to the exclusive formation of bicarbonates by CO_2 hydrolysis. Nevertheless, the regeneration cost of tertiary amines is significantly lower than the regeneration cost of primary amine [9].

In the past few years, mixed alkanolamines have received increasing attention. In most cases, the mixtures contain N-methyldiethanolamine (MDEA) as the base amine with the addition of one or two more reactive amines such as monoethanolamine (MEA) or diethanolamine (DEA) has been widely proposed [4]. The principle of such an aqueous blend with a tertiary amine is based on the relatively high rate of reaction of CO_2 with the reactive alkanolamine combined with the low heat of reaction of CO_2 with the tertiary alkanolamine, which leads to higher rates of absorption in the absorber column [10]. Blended MDEA/MEA solutions have been widely investigated for several years [2, 11, 12, 13].

MDEA promoted piperazine (MDEA / PZ) has been used commercially and was patented by BASF to remove CO_2 in ammonia plants [14]. PZ is a cyclical amine which does not have hydroxyl group but consists of two nitrogen atoms in its molecular structure. It has been shown to be an effective promoter in MEA, MDEA, and potassium carbonate due to its rapid formation of carbamates with CO_2[5]. The rate constant of PZ was much higher than that of conventional alkanolamines such as MEA make it an effective promoter for CO_2 removal [15]. The addition of small amounts of PZ to an aqueous solution of MDEA results in significant increase in the specific rate of absorption. In the past few years, there is a growing

interest among researchers to investigate PZ as an activator in MDEA solutions. Idem et al. [5] conducted experimental and simulation work at various concentration of MDEA/PZ, temperature and CO_2 loading to determine the reaction rate constant. Edali et al. [7] developed a 2D model for the blended amines MDEA/PZ using COMSOL software to study the concentration profiles of all the species considering both the radial and axial directions. It was revealed that PZ may be depleted when a loading of the solvent blend MDEA/PZ was greater than 0.015 mol/mol is exposed to CO_2 from the top of the laminar jet absorber. Closmann et al. [16] investigated the resistant of blended amine PZ/MDEA to the thermal and oxidative degradation. It shows that blended PZ/MDEA has higher thermal and oxidative degradation resistant than using pure amine, PZ or MDEA. Cullinane and Rochelle (2004)[17] studied the CO_2 absorption process in wetted-wall column using potassium carbonate and Piperazine (PZ). The addition of 0:6 M PZ to 20 wt. % potassium carbonate increased the rate of CO_2 absorption at 60 °C. PZ has a cyclic diamine structure that may favor rapid formation of the carbamates. As a mild base, it may catalyse the proton extraction in the reaction mechanism. Also theoretically, one mole of amine can absorb two moles of CO_2. The promoted potassium carbonate is expected to retain its low energy of regeneration, and the reaction of carbonate in bulk solution is expected to increase the absorption capacity. Svensson et al. [18] also stated that blended MDE/PZ required low the heat of absorption at regeneration phase. Due to this, interest in using hybrid solvents has increased to date.

There is a huge amount of experimental work done to study the CO_2 absorption process by amine absorbent. Recently, computer simulations are widely used all over the world including MD simulation. Molecular dynamic (MD) is a computer simulation technique of complex systems that is modelled at the atomic level. This computational technique is an effective method to discover more details about absorption process and also CO_2 capture [19].It will explain the molecular interaction and atomic in macroscopic and microscopic behaviours of the physical systems. This computational tool applies the concept of motion to molecules [20]. It is used to investigate the structure, dynamics, and thermodynamics of materials/chemical and biological system. MD simulation is initially started as the need to incorporate physical theory (electron and nuclei) to explain the details in chemistry [21]. Besides that, MD simulation offers a systematic and more accurate, calculation that gives results closer to the actual absorption process [22]. MD simulations is also used to explain the theory in chemistry studies for the microscopic behaviour at the nano-scale, such as diffusion, [23]. It also helps in saving the experimental

time and cost [24]. The understanding of fundamental in chemistry at the molecular level gives benefit in the study of the removal of CO_2.

Despite of more attention given for blended MDEA/PZ, the mechanism involved in absorption of CO_2 not well known. The aim of this study is to provide more insights into the absorption of CO_2 into aqueous solutions containing PZ and MDEA from molecular level point of view. Researches regarding to this process at molecular level are not well established since most of them focusing more at macro-scale level.

Molecular Dynamic Simulation

Molecular dynamic (MD) simulation approach is used in this study to investigate the molecular interaction at microscopic behaviour in amorphous box. Molecular dynamics model the motion of some group of particles (e.g., atoms) by solving the classical equations of motion which provides information on system dynamics in the atomic scale. MD simulation study of amine-based absorption for CO_2 capture were performed using Material Studio version 7.0 software on HP Z400 workstation with 8 GHz dual core processor.

Material studio software was supplied by Accelrys [25]. Setting parameter used in this simulation was atom based summation method (for geometry optimization), Ewald summation method (for equilibrium and production phase), COMPASS force field (for energy interatomic potential calculation), and velocity Verlet algorithm (for time integrator algorithm calculation). COMPASS is condensed-phase optimized molecular potentials for atomic simulation studies. COMPASS was suitable to be used for inorganic gas molecule, polymers and organic molecule. COMPASS force field is adds to the cross coupling term for the prediction of structural variation and vibration frequencies [26]. Verlet algorithm from Taylor expansion is used to calculate the velocity explicitly which may affect the simulation with constant pressure. This allows the usage of relatively long time steps duration as the position (r), velocities (v), and acceleration (a) are calculated at the same time with high precision. Besides this, the capability to conserve energy with numerically stable and time reversible properties becomes the reason for the software developer to use this algorithm [27]. The Verlet algorithm was used for the calculation of the atomic motion. Procedures for MD simulation involved four main steps. The first step was sketching and optimising the molecular structure. All interaction parameters were decided through a suitable force field. Second step was the creation of simulation box, followed by equilibrium and production phase simulation and lastly was trajectory output analysis.

The MD simulation was started with replicating the structure of actual molecule. The structure must be

accurate and similar with the real structure. Three dimensions (3D) atomisation of the actual structure molecule were downloaded from Royal Society of Chemistry database [28]. The advantage of using molecular structure obtained from this database was to prevent error in the sketches. A 3D molecule structure was used in this simulation because it involved a movement of the molecule and required in MD simulation. Geometry optimisation step was carried out on each of the molecule to ensure the stability of molecular geometry to be used in further simulation steps. The force field used in optimization step is Forcite calculation. Forcite calculation used in this simulation because capable to calculate the dynamics simulations, energy and geometry optimization. This Forcite calculation allow to analyze simple properties such as density variations and also complex properties such as dipole autocorrelation functional [25].

The creation of simulation box involved two steps i.e. box creation and energy minimisation. The simulation box was constructed using the amorphous cell calculation model in Material Studio software. The cubic periodic boundary condition was enabled to overcome the surface effect. The size of simulation box depended on the amount of molecules inserted. The simulation box size should be chosen correctly because the dimension and fluctuation of the box will be observed through simulation run [27]. Once the simulation box was created, this model was simulated for box energy minimisation. *Smart Minimize* module was selected for energy minimisation step and the convergence was set at fine level while the maximum iteration was set up to 10,000.The purpose of minimisation step was to minimise the energy of structure in the amorphous box and to correct the unrefined molecular structure with distorted bond angles and lengths or with steric clashes between atoms [29].

The equilibrium phase is simulated at constant NVE (number molecules, volumes, and total energy) ensemble for 200 ps with random initial velocities. The number of time steps between each output was 1 fs. The purpose of equilibration step was to ensure the system configuration was stable with energy conservation. The equilibrium phase was also known as molecular relaxation. Then, the simulation process was continued in the production phase under constant canonical ensemble, NVT (number of moles, volume and temperature) for 1 ns and a time step of 1 fs. The time step employed in MD simulation is 1 fs because in this simulation was run using the Verlet algorithm calculation. This algorithm calculation was used to calculate the positions and velocities of all atoms. Therefore, generally the time step was set to 1 fs which is very small and it is represent to bond stretching motions of C-H bonds vibration [30]. The final structures

were obtained from the trajectory output for analysis when the simulation under NVE and NVT ensembles were completed. Radial distribution function (RDF) results were used to analyse the final structure and its molecular interactions.

The RDF analysis for blended MDEA/PZ solution for CO_2 absorption is conducted through two system of interest i.e binary and tertiary. The binary system will explain the interaction between amine and water molecule while tertiary system used to determine the interaction between amine and CO_2 molecule. Binary MDEA/PZ blended system consisted of 10 wt% of PZ, 30 wt% of MDEA, and 60 wt% of water. Meanwhile for tertiary MDEA/PZ blended system comprised of 15 wt% of PZ, 30 wt% of MDEA, 50 wt% of water, and 10 wt% of CO_2. The temperature and pressure are kept constant at $40^{\circ}C$ and 1 atm, respectively. Table 1 shows the number of molecules and density specified in Material studio software. Figure 1 shows the molecular structure of amine, water and carbon dioxide used this simulation.

The density of mixture was calculated with two (2) steps. First, weight percent of solution was based on literature and done the conversion of mass of molecule to particles. Second, density mixture was calculated follows Equation 1 where ρ_i is density for species i and x_i is number of particles for species i. Density of liquid mixtures. i is species of liquid and x is number of particles. The density values were taken from 'Thermodynamic Properties of Chemical and Hydrocarbon' book based on specific temperature used.

$$\sum \left(\rho_i \times \frac{x_i}{x_{total}} \right) \qquad (1)$$

Results and Discussion

The intermolecular interaction of blended MDEA/PZ with water and CO_2 are analyse in terms of radial distribution function (RDF) analysis. The RDF determined the probability of intermolecular interactions occurred between one molecules of interest with the neighbouring molecule at a given distance, r from a central molecule. Strong intermolecular interaction is identified when a high value of g(r) is observed at a small distance of r. The binary system used to explain the interaction between amine and water molecule while tertiary system to determine the interaction between amine and CO_2 molecule. RDF plot shows the relationship between r which is the distance between atom pairs in each of the trajectory distance of atom with other neighbouring atom and g(r) is the tendency of atom to

interaction/probability to have interaction between atoms.

Table 1: Number of molecules and density for blended MDEA/PZ solution.

Density mixture for amine solution system (g/ml)	0.9942		
Number of molecule for amine solution system	MDEA	PZ	H_2O
	30 wt%	10 wt%	60 wt%
	60	30	870
Density mixture for reaction between amine and CO_2 system (g/ml)	0.9886			

Number of molecular for reaction between amine and CO_2 system	MDEA	PZ	H_2O	CO_2
	30 wt%	10 wt%	50 wt%	10 wt%
	44	20	478	40

(a) Methyl Diethanolamine (MDEA)

(b) Piperazine (PZ)

(c) Carbon Dioxide (CO_2)
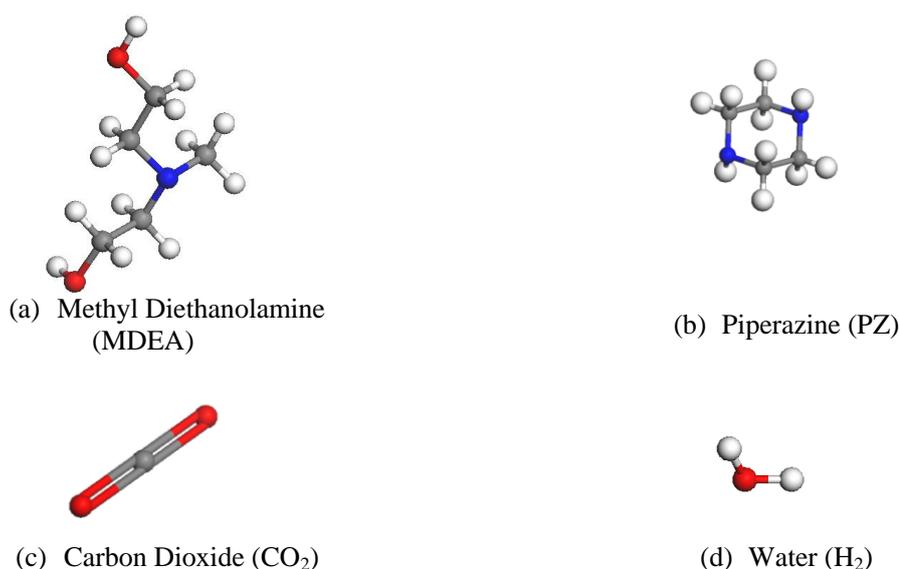
(d) Water (H_2)

Figure 1: Molecular structure of (a) methyl diethanolamine (MDEA), (b) piperazine (PZ), (c) carbon dioxide (CO_2), and (d) water (H_2O) used in MD simulation.

Intermolecular interaction of amine with water for pure and blended amines system

Binary system which consists of amine and water molecules is simulated to analyse the potential of intermolecular interaction between both molecules. Table 2 shows the summary data of RDF results which extract from Figure 2 and 3 shows the RDF results for binary system using pure MDEA and blended MDEA/PZ.

The main reason for performing this simulation was to investigate the distribution of MDEA and PZ in water. Table 2 shows the intermolecular interaction between pure MDEA and PZ and blended MDEA/PZ with water without the CO_2. It is clearly seen that the intermolecular interaction of HO_{mdea}-O_{water} for pure MDEA system was higher than the blended MDEA/PZ. At the same distance of 1.75 Å, the tendency for the interaction to happen for pure MDEA and blended MDEA/PZ were $g(r)$ = 2.2293 and 1.6574, respectively. It can be concluded that water had stronger intermolecular force of polar bond with HO_{mdea} in pure MDEA compared to blended MDEA/PZ (34.51% increment), due to the MDEA structure that had two –OH bonds and it more tendency the intermolecular interaction with water to form hydrogen bond. But in blended MDEA/PZ, the presence of PZ with lack of hydroxyl group affected the tendency of HO_{mdea} interaction with water. No hydrogen atom was directly connected to the nitrogen atom in the molecular structure, thus it cannot generate carbamate ions. This justification was based on molecular structure of MDEA and PZ in methodology

section. Where MDEA has two hydroxyl group (-OH) and PZ does not has hydroxyl group (-OH).

It contrary with amino group, the intermolecular interaction of N_{mdea}-H_{water} and N_{pz}-H_{water} in blended

MDEA/PZ was higher compared to pure MDEA and PZ.

Table 2: Summary data of RDF result for binary system of MDEA and PZ, and blended MDEA/PZ system.

Binary				
	HO_{mdea}-O_{water}	N_{mdea}-H_{water}	HO_{pz}-O_{water}	N_{pz}-H_{water}
MDEA	1.75, 2.2293	4.75, 1.1107	-	-
PZ	-	-	-	5.75, 1.0255
MDEA+PZ	1.75, 1.6574	4.75, 1.1936	-	5.75, 1.0323
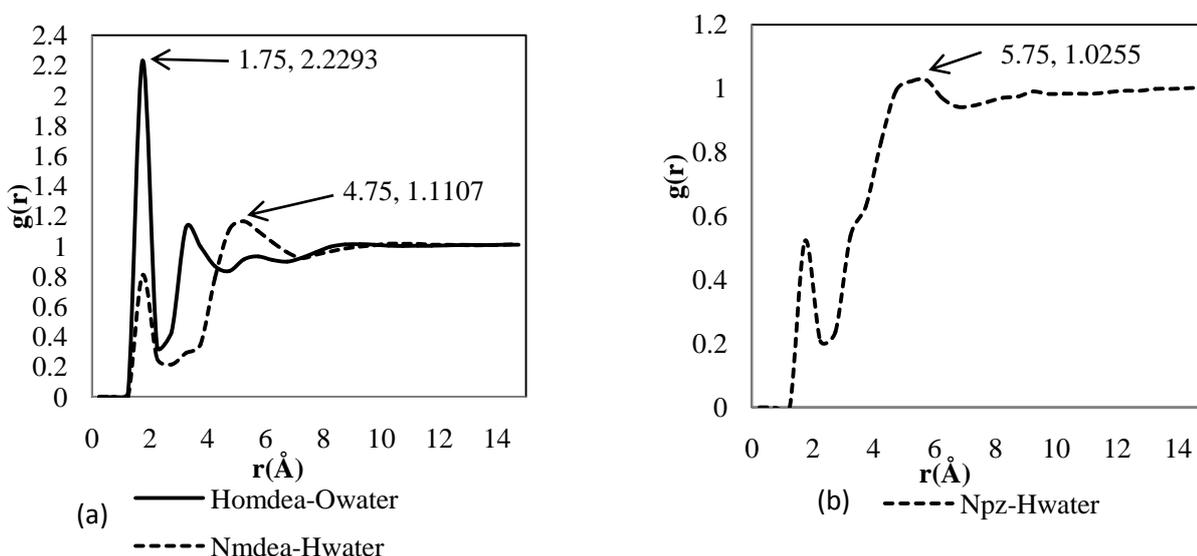
Figure 2: Intermolecular interactions of amine and water in binary system using (a) MDEA and (b) PZ solution.
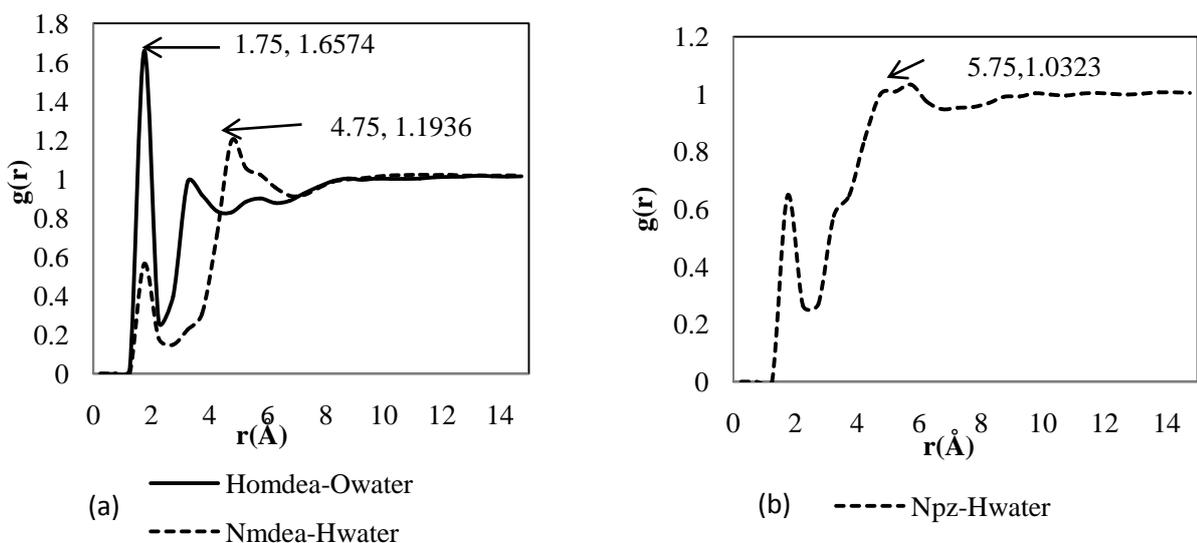
Figure 3: Intermolecular interaction of (a) MDEA and water and (b) PZ and water for binary system of blended MDEA/PZ.

As depicted in Table 2, the $g(r)$ value of N_{mdea}-H_{water} for pure MDEA system was 1.1107 and for blended MDEA/PZ was 1.1936 (7.46% increment), at the same

distance of 4.75 Å. Whereas, $g(r)$ value of N_{pz}-H_{water} for pure PZ system was 1.0255 and for blended MDEA/PZ was 1.0323 (0.66% increment), at the same

distance of 5.75 Å. The presence of PZ in the solution enhanced the interaction of N_{mdea} with water. Table 3 show the summary data of RDF result which extract from Figure 4 and 5 shows the RDF result for intermolecular interaction between pure MDEA and PZ and blended MDEA/PZ in tertiary system with CO_2 in solution.

Table 3: Summary data of RDF result for tertiary system of MDEA, PZ, and blended MDEA/PZ system.

|	Tertiary			
	HO_{mdea}-O_{water}	N_{mdea}-H_{water}	HO_{pz}-O_{water}	N_{pz}-H_{water}
MDEA	1.75, 2.6546	4.75, 1.2557	-	-
PZ	-	-	-	5.75, 1.0926
MDEA+PZ	1.75, 2.7057	4.75, 1.8805	-	5.75, 1.1562
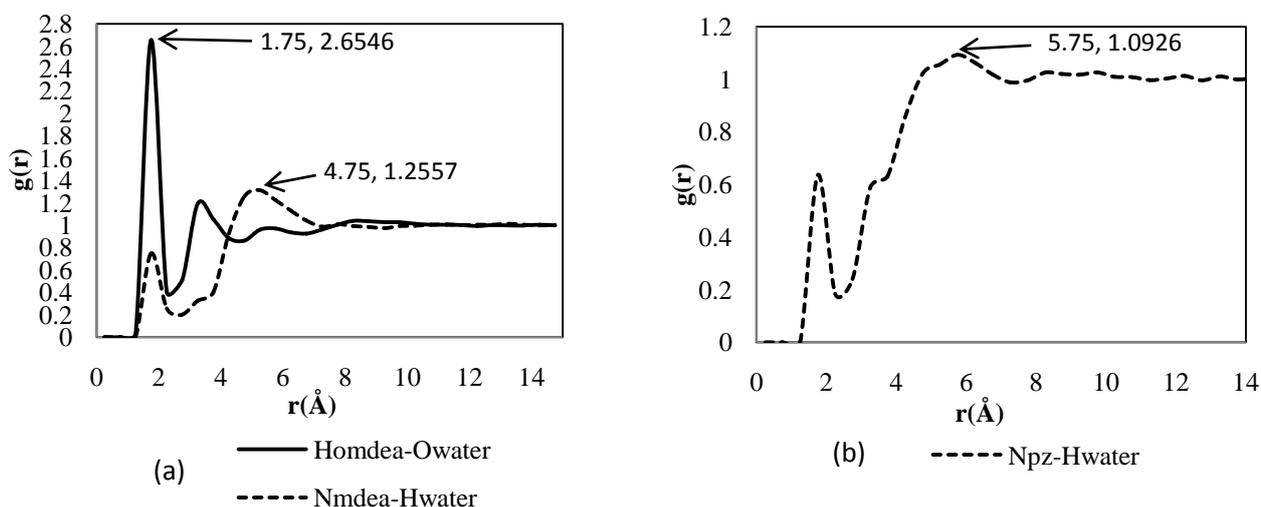
Figure 4: Intermolecular interactions of amine and water in tertiary system using (a) MDEA and (b) PZ solution.
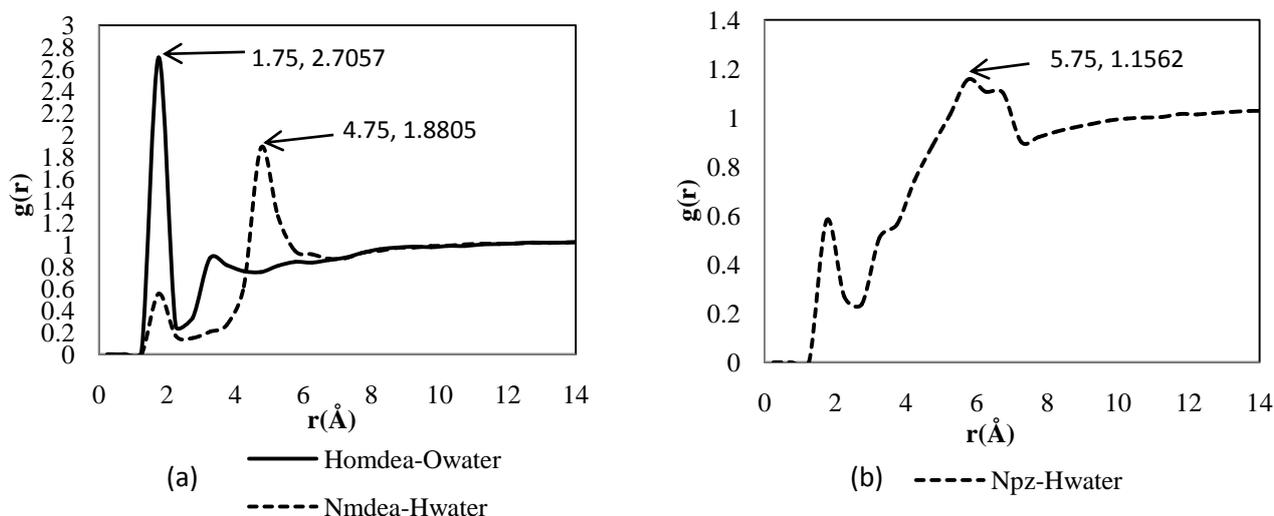

Figure 5: Intermolecular interaction of (a) MDEA and water (b) PZ and water for tertiary system of blended MDEA/PZ.

Based on RDF results, in the presence of CO_2, MDEA and PZ solution had strong intermolecular interaction with water compared to MDEA and PZ solution alone (without CO_2 molecules). For example, at same distance of 1.75 Å, the tendency for the intermolecular interaction to occur on binary and tertiary systems of HO_{mdea}-O_{water} for blended MDEA/PZ were 1.6574 and 2.7057 (63.25% increase), respectively. The addition of small PZ was capable to increase the solubility of CO_2 in amine solution [27]. The similar behaviour was

observed for blended MDEA/AMP in previous discussion.

For tertiary system, both hydroxyl and amino groups of blended MDEA/PZ showed strong intermolecular interaction with water compared to pure MDEA and PZ. This behaviour indicates that mixture of MDEA/PZ was stronger reactive with CO_2 compared to pure amine. For example, at a distance of 5.75 Å, the intermolecular interaction of amino group of PZ for pure PZ and blended MDEA/PZ were 1.0926 and 1.1562 (5.82% increase), respectively. PZ was able to activate the reaction of MDEA with CO_2 [31]. The presence of two nitrogen atoms in PZ increased the uptake of CO_2 to MDEA.

However, the strength of intermolecular interaction for N_{pz}-H_{water} was weaker than hydrogen bonding of HO_{mdea}-O_{water} and N_{mdea}-H_{water} where the result RDF was 1.0926 at a distance of 5.75 Å. PZ as aromatic amine has lone pair electrons which conjugated and shares an electron in the benzene rings. From this, the possibility to form hydrogen bonding was reduced that led to low solubility in water.

Based on the explanation, there was a significant effect on the diffusion of amine in water with the addition of CO_2. This is good because for tertiary amine, it cannot directly react with CO_2, but with presence of water can driven CO_2 to become bicarbonate ion. Based on Lu et al., 2005[32], blended MDEA/PZ shows good performance for CO_2 absorption compared to pure MDEA solution up to 99%. This study also shows that the small quantity of PZ was capable to improve the mass transfer in membrane for CO_2 gas absorption process.

Intermolecular interaction of amine with CO_2 for pure and blended amines system

In tertiary system, CO_2 molecules are added to the amine solution. The RDF results for tertiary system used to explain how the existence of CO_2 molecule will affect the intermolecular interaction in amine solution presented in binary system and dissolution of CO_2 into amine solution. Table 4 shows the summary data of RDF results which extracted from Figure 6 and 7 shows the graphical results for intermolecular interaction between amine and CO_2 for MDEA, PZ, and MDEA/PZ system.

The results for the study on tendency of CO_2 towards amine solution were displayed in Table 4. From the RDF result, the values of r and $g(r)$ for pure MDEA system were (3.75, 1.1488) and (5.25, 1.5158) for O_{mdea}-C_{co2} and N_{mdea}-C_{co2}, respectively. The results show an increment after a small quantity of PZ was added into MDEA, which were (3.75, 1.1883) and (5.25, 1.8766) for O_{mdea}-C_{co2} and $N_{mdea\text{-}Cco2}$, respectively. Again, the addition of PZ in MDEA solution could increase the strength of intermolecular

interaction between MDEA and CO_2. The absorption of CO_2 by MDEA solution was more efficient by the additional chemical reaction of PZ [32]. PZ as an activator was added to MDEA solution in order to accelerate the intermolecular interaction of MDEA with CO_2.

Based on Table 4, the distance for intermolecular interaction of N_{pz}-C_{co2} (4.25, 1.4911) was shorter than N_{mdea}-C_{co2} (5.25, 1.8766) because PZ was reacted first with CO_2. MDEA cannot react directly with CO_2 due to the lack of hydrogen atom at amino group. PZ was attracted and combined with CO_2 then transferred to MDEA rapidly [32]. The reaction of PZ with CO_2 produced carbamate that subsequently reacted with MDEA to form bicarbonate. PZ was acted as a promoter to activate the MDEA to absorb CO_2. The reaction of CO_2 and PZ was in parallel with the reaction of CO_2 with MDEA in the condition of rapid pseudo-first-order reaction [6].

Previous studies were carried out to find the CO_2 absorption capacity [31]. The findings show that 30 wt % of PZ was the highest capacity up to 1.06 mole CO_2/mole amine compared to other amines such as MDEA. The molecular structure of PZ with two nitrogen atoms was expectedly doubled the CO_2 absorption capacity. Another study about membrane gas absorption (MGA) process using hollow fibre contactor, the average overall mass-transfer coefficient of blended MDEA/PZ was 2.25 times higher than pure MDEA [32]. PZ plays an important role for accelerating the absorption process of CO_2 in MDEA solution. Because PZ is a cyclic secondary diamine, its efficiency is attributed to its cyclic diamine structure that may favour rapid formation of carbamate with CO_2. As a mild base, it may serve to catalyse proton extractions in the reaction mechanism. Also, the molecule can theoretically absorb 2 moles of CO_2 for every 1 mole of amine [17]. Moreover, Svensson et al. (2013)[18] also stated that blended MDE/PZ required low the heat of absorption at regeneration phase. Due to this, interest in using hybrid solvents has increased to date.

The intermolecular interaction comparison of PZ and MDEA with CO_2 as illustrated in Figure 5 demonstrates that, PZ molecules have higher probability of interaction than MDEA.

The highest probability of intermolecular interaction for MDEA with CO_2 occurred at 5.25Å distance of r. Based on the reaction mechanism reported by Lu et al. [32] as shown in equation 2, 3 and 4PZ will react first with CO_2 to form PZ carbamate (PZCOO⁻) that subsequently reacted with MDEA to form bicarbonate (HCO$_3^-$). MDEA cannot react directly with CO_2 due to the lack of hydrogen atom at amino group.

Strong intermolecular interaction observed in this study perhaps leads to fast reaction of PZ with CO_2.

PZ has been reported as an effective activator which quickly reacts with CO_2 to form carbamate ion [15, 22]. Because PZ is a cyclic secondary diamine, its efficiency is attributed to its cyclic diamine structure that may favour rapid formation of carbamate with CO_2.

$$PZ + CO_2 \leftrightarrow PZ - CO_2 \tag{2}$$
$$PZ - CO_2 + H_2O \leftrightarrow PZCOO^- + H^+ \tag{3}$$
$$PZCOO^- + MDEA + H_2O \leftrightarrow MDEAH^+ + HCO_3^- + PZ \tag{4}$$
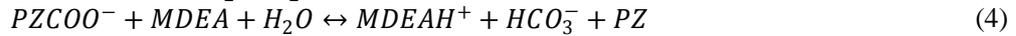
Table 4: Summary data of RDF result for reaction between amine with CO_2 on MDEA and PZ, and blended MDEA/PZ system.

|	Tertiary			
	O_{mdea}-C_{co2}	N_{mdea}-C_{co2}	O_{pz}-C_{co2}	N_{pz}-C_{co2}
MDEA	3.75, 1.1488	5.25, 1.5158	-	-
PZ	-	-	-	4.25, 1.0705
MDEA+PZ	3.75, 1.1883	5.25, 1.8766	-	4.25, 1.4911
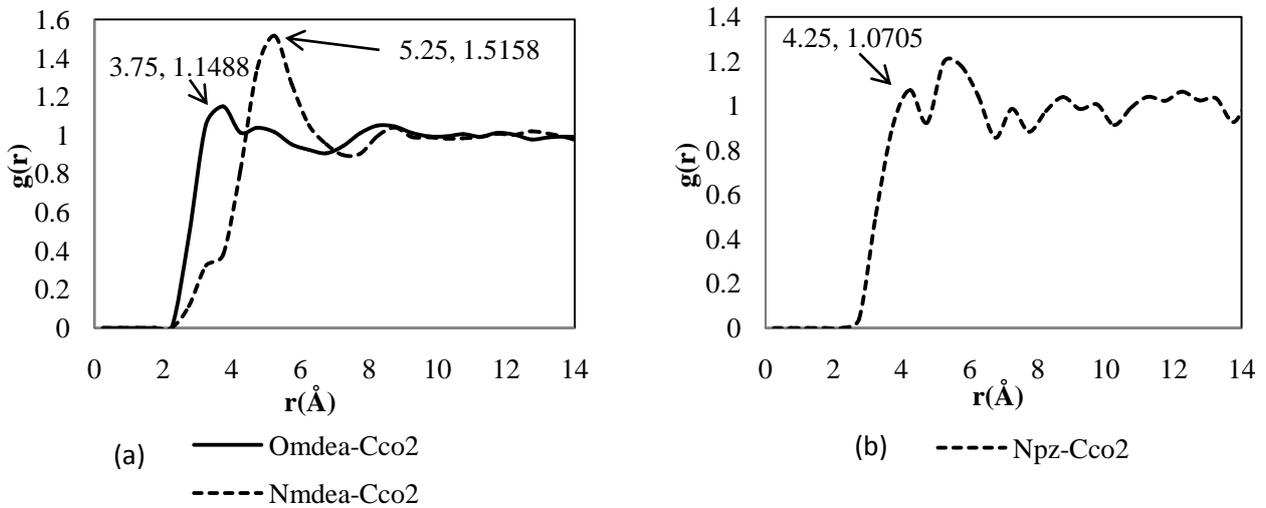
Figure 6: Intermolecular interaction of amine and CO_2 in tertiary system using (a) MDEA and (b) PZ solution.
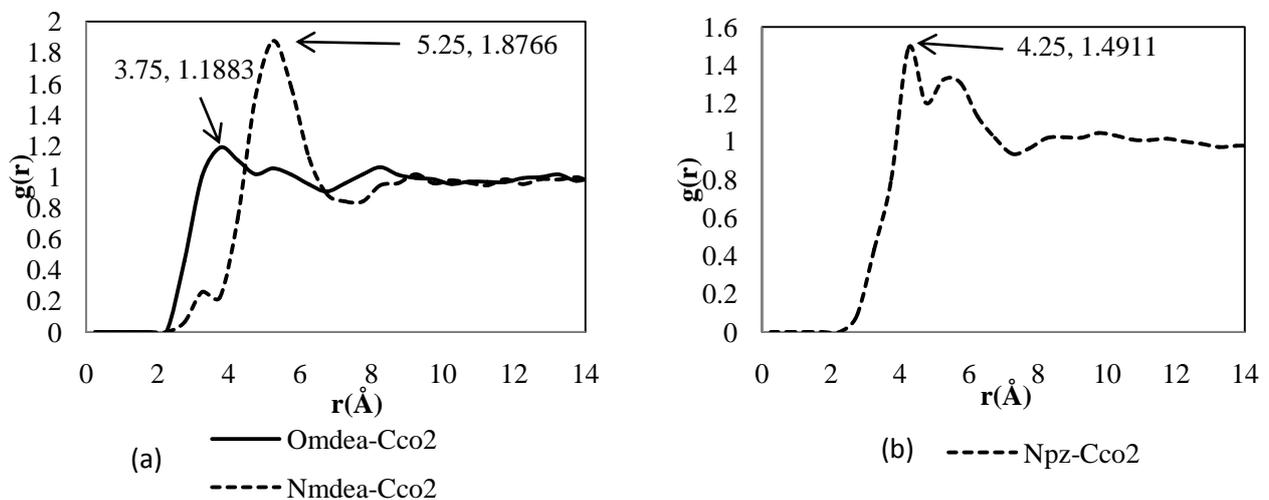

Figure 7: Intermolecular interaction of (a) MDEA and CO_2 and (b) PZ and CO_2 for tertiary system of blended MDEA/PZ.
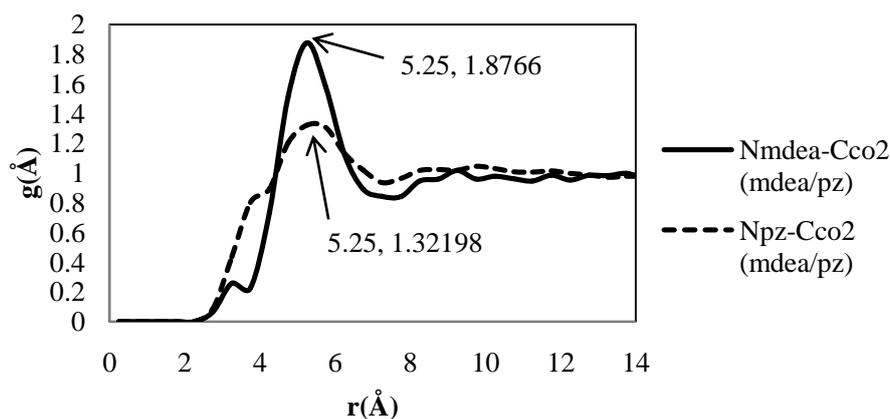
Figure 8: Intermolecular interaction of (a) MDEA and water (b) PZ and water for tertiary system of blended MDEA/PZ.

Conclusion

The outcome from this research can be applied as guideline to select solvent based on it characteristics which give significant effect to absorption process. This will help in improving the existing solvents and to be considering blended amine solvent in the future so that the performance of this process can be improved. The intermolecular interactions which describing the physical interaction among molecules shows the effect of molecular structure on CO_2 capture process. Strong intermolecular interaction between MDEA and CO_2 in blended MDEA/PZ system shows the significant effect of PZ in accelerating the reaction between MDEA and CO_2. The presence of activator amine, PZ, improved the intermolecular interaction of MDEA with CO_2. Research on molecular modeling of amine absorption process for CO_2 capture is proposed in this study to give insight about this process at molecular level to analyze the intermolecular interaction between CO_2 and amine solution. The strength of intermolecular interaction will represent the effectiveness of absorption process. Better understanding on the solvent molecular structure and intermolecular interaction of solution mixture is crucial to improve CO_2 removal process using amine-based solvents to be more energy efficient, reduce losses and corrosion rates.

Acknowledgement

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