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Evaluation of CO_2 absorption performance by molecular dynamic simulation for mixed secondary and tertiary amines

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ABSTRACT

CO_2 emission to the atmosphere is the most prominent cause of climate change and a major risk to environmental health. Although several techniques are very promising to reduce the CO_2 emission from central emission points, the CO_2 absorption by amines remains the most mature and reliable technology. Yet, there is more potential to improve absorption performance by choosing suitable solvents. Thus, the present research is intended to explore a better solvent combination for CO_2 absorption by adopting the amine absorption process using molecular dynamic simulation. The study is designed to compare the intermolecular interactions of N—C and N—H bond between single 2EAE, DMAE (or 2DMAE), and blended solvent, i.e., 2EAE/PZ, 2DMAE/PZ with carbon dioxide and water and then to catch the effect of piperazine on these amines. The molecular dynamic simulations were performed by using the Material Studio application. The solvent concentration, 30 wt% under the condition of 313 K temperature at 0.1 MPa pressure, was taken for solvent systems. The results were interpreted by the Radial Distribution Function analysis. It was found that the blend of secondary and tertiary amines with piperazine 2EAE/PZ, DMAE/PZ reflect higher intermolecular interaction with CO_2 as compared to single DMAE & 2EAE. This finding shows that piperazine acts as a promoter on 2EAE and 2DMAE when interacting with CO_2.

1. Introduction

Carbon dioxide emission to the atmosphere is the major cause of climate change and a gradual increase in earth temperature, which is causing a serious threat to the world population as well as to economic development. In the recent past, global warming has shown its worse effects on climate change and environmental health (Chen et al., 2019). According to World Energy Outlook (WEO2013) projects, global emission of CO_2 from the combustion of fuels will continue to rise from 31.3 Gt in 2011 to 37.2 Gt in 2035 unless tremendous efforts are made to control the CO_2 emission (IEA, 2013). Therefore, it is need of the day to cut down the CO_2 emission from generated flue gas. Carbon capture and storage (CCS) is considered as an attractive approach to reduce the CO_2 emission and is expected to play a vital role in CO_2 emission mitigation in foreseeable future until the development and applications of low carbon or even zero-carbon energy technologies can truly be achieved (Schiermeier et al., 2008). The CCS chain comprises three steps: capture, transport, and storage. So far, capture technologies can be divided into three main strategies: pre-combustion capture, post-combustion capture, and oxy-combustion capture (Tan et al., 2016; Liang et al., 2016). Post-combustion carbon dioxide capture by chemical absorption using alkanol amines is considered as state of the art technology because of direct and easy installation to the existing power plants (Wang et al., 2011).

The main challenge in chemical absorption method is to find a suitable and efficient solvent that satisfy the important parameters, such as high absorption capacity with fast reaction rate, low heat energy to regenerate the solvent, low corrosion and low degradation (Yamada et al., 2013; Conway et al., 2014). To achieve these essential properties, individual amines are proposed to be blended to take the advantages of each pure amine (Muchan et al., 2017). Amines, especially alkanol amines, are particularly common due to their relatively low cost, high capacity, and fast reaction rate (Orozco et al., 2014). There are few examples for these blends, such as MEA/MDEA (primary and tertiary amine), AMP/DEA (hindered and secondary amine), DEA/MDEA (secondary and tertiary amines), etc. Other examples include PZ piperazine (cyclic diamine), EDA, and DETA multi-amines (ethylenediamine and diethylenetriamine) (Muchan et al., 2017; Zhang et al.,

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2014).

Mainly there are three important parameters to select a suitable solvent for CO_2 absorption. First is the solubility of the solvent with CO_2. Second, the regeneration energy of solvent in the desorption process and, third is the reaction kinetics of amine with carbon dioxide. As the reaction kinetics directly affects the rate of absorption, which finally affects the equipment size, such as the column's height of the absorber (El Hadri et al., 2017). A lot of efforts are being made to increase the reaction kinetics of the solvents to reduce the solvent circulation rates, which in result reduces the equipment size and thus reduces the cost of capture plant (Sema et al., 2019; Davison, 2007).

El Hadri et al. (2017) investigated the thermodynamics and kinetic properties of different aqueous solutions (primary, secondary & tertiary) for CO_2 absorption and calculated CO_2 loading, absorption heat and kinetics of the reaction. It was observed that absorption capacity and absorption heat for tertiary amine favors the use of tertiary amines for CO_2 absorption, but the slow absorption rate of tertiary amines makes them unfeasible for wide adoption. It was also studied that 2EAE secondary amine has good reaction kinetics, and it was also suggested to use 2EAE as an alternative to MEA in the CO_2 capture process. Liu et al. (2019) performed laboratory experiments to explore the energy for primary and secondary amines. Molar Gibbs energy change and molar reaction enthalpy were estimated to evaluate the suitable absorbents for carbon dioxide capture, and finally, the study suggested two promising absorbents (i.e., EAE and MAE) for CO_2 removal. Ismael et al. (2009) conducted the simulation work to study the mechanism of carbamate formation by absorption of CO_2 in AMP (2-amino- 2-methyl-1- propanol) using DFT. The results of that study revealed that the role of water as a basic reactant, leading to the stable intermediate formation. Harun and Masiren (2017) did the molecular dynamic simulation to check the intermolecular interaction of MDEA/PZ blended amine. In simulation methodology, COMPASS was used as a force field, and Ewald was used as a summation method. The result of this study showed that MDEA has low intermolecular interaction than blended MDEA/PZ. Furthermore, PZ acts as an activator to promote the intermolecular interaction between MDEA and CO_2.

Ahmad et al. (2018) carried out the simulation study to categories the solvent with low regeneration energy and maximum efficiency for carbon dioxide absorption and suggested that 2EAE and DMAE should be considered as promising solvent candidates for CO_2 capture. Yu et al. (2013) conducted a study to optimize the amine mixing solution design for CO_2 capture by molecular dynamic simulation. This study characterized the transport properties of multi-amine and calculated the overall synergy in ternary, quaternary, and quintuple amines. The result indicates that the overall synergy in ternary amines was found to be better than in quaternary and quintuple amines. Zhang et al. (2018) conducted the simulation work on binary solution of AMP/DEA, MEA/PZ with ab initio calculation by using DFT to check the chemical enhancement of CO_2 capture. The results show that PZ presents the lowest forward energy barrier and second-lowest backward energy barrier in zwitterion formation and MEA + COO- based reactions have good absorption property while AMP + COO- based one favors the desorption process.

The existing literature indicates that a lot of efforts have been made to find a suitable and efficient solvent system that has all the qualities, i.e., higher absorption capacity, low absorption heat, fast reaction rate, and low regeneration energy, etc. Although a number of solvents are suggested in literature, but, the identification of most promising solvents remain unsolved. Thus the current study intended to find a suitable and efficient solvent system for CO_2 absorption. To select an absorbent for CO_2 absorption is very technical and significant due to the different properties such as absorption capacity, the reaction rate of amines with CO_2, energy consumption in operating process, viscosity, and corrosiveness (Bougie and Iliuta, 2012; Damartzis et al., 2016). In the present study, the selected solvents are, i.e., 2-ethylamino ethanol (2EAE), 2-dimethylamino ethanol (2DMAE), and piperazine (PZ). 2EAE is a secondary alkanol amine, 2DMAE is a tertiary alkanol amine whereas, piperazine (PZ) is a secondary, cyclic di-amine. The solvents were selected on the bases of their advantages as described in the existing literature, such as; 2EAE has higher absorption capacity and low heat of absorption than MEA (El Hadri et al., 2017). The desorption enthalpy of 2EAE (104.06 kJ/mol) is near to that of MEA (97.43 kJ/mol), and reaction kinetics of 2EAE is very close to MEA. Furthermore, 2EAE has high energy efficiency for CO_2 removal, which can make 2EAE as a potential absorbent for industrial applications (Liu et al., 2019; Ahmad et al., 2018). 2DMAE is a tertiary amine and has a relatively good absorption rate ($\alpha > 0.7$) than other tertiary amines, i.e., MDEA and TEA. Moreover, 2DMAE has low absorption heat ($\Delta H <$ 70 kJ/mol) and low enthalpy of desorption (83.78 kJ/mol) than MEA (Ahmad et al., 2018; El Hadri et al., 2017). Piperazine (PZ) is a famous secondary cyclic di-amine and has a higher rate of absorption as well as higher resistance to degradation as compared to MEA (Freeman and Rochelle, 2012). Due to these important qualities, PZ is considered as a new benchmark for CO_2 capture (Rochelle et al., 2011; Rabensteiner et al., 2015). Other studies such as (Derks et al., 2006; Bishnoi and Rochelle, 2000), also suggested that piperazine has a unique faster reaction rate. Piperazine, when mixed with a tertiary and hindered amine, also shows faster reaction rate and good carbon dioxide cyclic capacity as compared to conventional solvent MEA. Moreover, it is more stable to heat and less volatile in amines (Du et al., 2016; Sun et al., 2005). Piperazine has also been used for blending to increase the reaction rate and absorption capacity (Muchan et al., 2017). Mixing piperazine with 2EAE and 2DMAE can help to increase the reaction rate and absorption capacity of these solvents.

Recently, computer-based simulation is widely used in all over the world in different research fields. The present study will adopt molecular dynamic simulation to analyze the intermolecular interaction during the process of absorption. The Molecular dynamic is a computer simulation technique of a complex system that is modeled at the atomic level. This computational technique is an efficient method to discover more details about the process of absorption and CO_2 capture (Maginn and Elliott, 2010). This technique helps to explain the physical system of atomic and molecular behavior of interaction in microscopic and macroscopic systems and also explains the motion of molecules in the system (Lewars, 2016). The advantages of molecular dynamic simulation (MD) include that it can be used to observe the structure of a system, dynamics, thermodynamic properties of the material, and to observe the chemical and biological system. It was initially started to study the physical theory in chemistry. In addition to that, MD simulation offers an ordered and more accurate calculation that gives results closer to the actual process of absorption (Jensen and Truhlar, 1987; Xing et al., 2013). It also saves time and cost, as researchers can find an efficient and suitable solvent without buying expensive equipment experiments and also saves time for experiments (Charpentier, 2002). Overall molecular dynamic simulation is a powerful and attractive tool to check the absorption process at molecular level. Radial distribution function (RDF) will be used to analyze the molecules which are provided by molecular dynamic simulation and computational method will be used to do calculations.

Thus the main aim of this study is to find a better solvent combination for CO_2 absorption by exploring the strongest intermolecular interaction of amines with CO_2 and water and to explore the effect of piperazine in selected secondary and tertiary amines. In that perspective, the three aspects of the present research are the main contribution to the existing research; first, the current study adopted the computational tool like molecular dynamic (MD) simulation to study the behavior of molecules during the absorption process. Secondly, the present study used blended and non-blended secondary and tertiary amines solvents to explore the solvent system with higher intermolecular interaction so that the solvent system can be selected for experimental studies. And the solvent system with higher intermolecular interaction will facilitate the absorption process and will

provide the information about the reaction of amines with CO_2 (Masiren et al., 2016b; Harun and Masiren, 2017). Third, the study used an unexplored blended mixture (2EAE/PZ and DMAE/PZ) of amines in contrast to other studies that blended PZ with AMP, MEA-MDEA, and MDEA (Xie et al., 2013; Zhang et al., 2017; Harun and Masiren, 2017). Based on the best knowledge of the author, no (MD) study is conducted before for these blend systems. Finally, the findings will help to select the most promising amines for laboratory experiments and for industrial use to protect the environment by reducing carbon emissions to the atmosphere.

2. Theory

2.1. Reaction mechanism for 2EAE

A lot of studies have been carried out to explore the reaction mechanism for primary, secondary, tertiary, and hindered amines (Liu et al., 2019; Ahmad et al., 2018, Sodiq et al., 2018). The primary and secondary amines have a higher reaction rate for CO_2 absorption, which produces zwitterion as given in Eq. (1), and then it transfers a proton to form carbamate as Eq. (2). Their maximum possible CO_2 loading is 0.5 mol of CO_2/mole of amine (two amine molecules react with one CO_2). At the high pressure, the carbamate could be hydrolyzed to form a free amine and bicarbonates, and later this free amine will again react with CO_2 as given in Eq. (3) (Quang et al., 2013). The complete reaction mechanism is presented by Eq.s (1),(2) and (3).

$$R_1R_2NH + CO_2 \leftrightarrow R_1R_2NH^+COO^- \quad (1)$$

$$R_1R_2NH^+COO^- + R_1R_2NH \leftrightarrow R_1R_2NCOO^- + R_1R_2NH^+ \quad (2)$$

$$R_1R_2NCOO^- + H_2O \leftrightarrow R_1R_2NH + HCO3^- \quad (3)$$

2.2. The reaction mechanism for DMAE

Dimethylaminoethanol is tertiary amines. The reaction mechanism of CO_2 with tertiary amine is different from primary or secondary amines. For tertiary amines, the maximum CO_2 loading could be one mole of CO_2 per mole of amine (one molecule of amine reacts with one molecule of CO_2) with the formation of bicarbonate (Eq.s (4,5)). Although the tertiary alkanol amines have higher CO_2 loading but they have low reactivity with CO_2 as compared to primary or secondary amines (Muchan et al., 2017; Donaldson and Nguyen, 1980).

$$CO_2 + H_2O \leftrightarrow H^+ + HCO3^- \quad (4)$$

$$R_1R_2R_3N + CO_2 + H_2O \leftrightarrow R_1R_2R_3NH^+ + HCO3^- \quad (5)$$

2.3. The reaction mechanism for Piperazine (PZ)

Piperazine is a cyclic secondary di-amine. It forms carbamate ion, zwitterion as well as protonated carbamate when reacts with CO_2. The reaction mechanism of piperazine with carbon dioxide is given below in Eq.s (6),(7) and (8) as represented by (Derks, 2006; Masiren et al., 2016b).

$$CO_2 + 2PZ \leftrightarrow PZCOO^- + PZH^+ \quad (6)$$

$$CO_2 + PZCOO^- + B \leftrightarrow PZ(COO^-)2 + BH^+ \quad (7)$$

$$CO_2 + PZH^+ + B \leftrightarrow H^+PZCOO^- + BH^+ \quad (8)$$

3. Simulation methodology

Material Studio (MS) software 2017, provided by BIOVIA, was used for simulation. The simulation methodology for CO_2 absorptions process can be segregated into six steps, i.e., first, the molecular structure sketch, Royal Society of Chemistry database, was used to get the structures of selected molecules. Three-dimensional structures (3D) were obtained to replicate the true behavior of molecules based on the actual absorption process (ChemSpider-Database, 2019). In the second step, the energy minimization for all selected molecules was carried out for each structure to get a stable structure in forcite. The basic purpose of using forcite calculation is its capacity to calculate dynamic simulation, energy, and geometry optimization. Furthermore, forcite calculation allows analyzing simple properties, i.e., density variation and complex properties such as dipole autocorrelation functional. The third step involves two parts, (I) the construction of a simulation box and (II) energy minimization of the simulation box. The simulation box was created in the amorphous cell. The size of the box depends upon the number of molecules inserted. In the simulation process, the dimensions and fluctuation of the box will be observed, so the size of the box should be chosen carefully (Farmahini, 2010). Amorphous box construction involves the density calculation according to the weight percentage of different selected solvents. Tables 1 and 2 show the calculations of the number of molecules and density specified in Material studio software, and Eq. (9) represents the density calculation. The energy of the simulation box was minimized before starting the dynamics at the equilibrium and production phase. The purpose behind the energy minimization of the simulation box is to get all the atoms in the stable configuration and to correct the unrefined molecular structures (Adcock and McCammon, 2006). The fourth step is dynamics at equilibrium under constant NVE (number of molecules, volume, and total energy) at 200 ps with random initial velocities and a time step of 1 fs. The main aim of this process is to get a stable system configuration with energy conservation. This equilibrium phase is also known as molecular relaxation (Malik et al., 2010). COMPASS and Ewald models were used for force field and summation method calculation, respectively (Higashi and Tamura, 2010). COMPASS (Condensed phase Optimized Molecular Potential for Atomic Simulation Studies) is an effective force field, and as a general, it is known as all atoms force field. It is based on ab initio empirical parameterization techniques (Qiang et al., 2013). The fifth step is the dynamics at the production phase under constant canonical ensemble NVT (number of molecules, volume, and temperature). The time step of 1 fs was selected to ensure all the molecules in the simulation box do not overlap each other (Higashi and Tamura, 2010). The sixth and last step is the radial distribution function

Table 1
Input parameters for 2EAE & blended 2EAE/PZ.

Density of mixture g/mL	0.97			
	2EAE	CO_2	H_2O	
Wt%	30 %	10 %	60 %	
No. of molecules	29	20	294	
Density of mixture g/mL	0.96			
	2EAE	PZ	H_2O	CO_2
Wt %	30 %	10 %	50 %	10 %
No. of molecules	58	20	478	39

Note: Author's Formulations and Tabulations. Wt% shows the weight percentage and No. represents the numbers. PZ stands for piperazine.

Table 2
Input parameters for pure DMAE & blended DMAE.

Density of mixture g/mL	0.97			
	DMAE	CO_2	H_2O	
Wt%	30 %	10 %	60 %	
No of molecules	44	30	441	
Density of mixture	0.96			
	DMAE	PZ	H_2O	CO_2
Wt %	30 %	10 %	50 %	10 %
No of molecules	86	30	716	58

Note : Author's Formulations and Tabulations. Wt% shows the weight percentage and No. represents the numbers.

(RDF) analysis of the final trajectory to check the intermolecular interaction between different atoms. Radial distribution function analysis was done for four types of amine, i.e. 2EAE, 2EAE/PZ, DMAE, and DMAE/PZ. The calculations used in Molecular Dynamic simulation and Radial Distribution Function RDF analysis are based on manual tutorial of Biovia Material Studio software (Biovia, 2017). Periodic boundary conditions are set of boundary condition which are used for approximating a large infinite system by using a small part called unit cell. Periodic boundary condition are implemented in y and z direction perpendicular to the stream wise x direction. The present study used fixed boundary conditions. While using fixed or periodic boundary condition, we also have to choose the geometry for the box surrounding system. In modelling of gas or liquid, the most useful way is to take the simplest box shape i.e to use the square (cube) box. thus, the present study took a cubic simulation box.

The density of the mixture was calculated with two steps (Harun and Masiren, 2017). First, the weight percentage of solution based on literature and then the conversion of the mass of molecules to particles. Second, the density of mixture was calculated based on Eq. (9),

$$\text{The density of mixture} = \Sigma(\rho_i \times \frac{x_i}{x_{total}} \tag{9}$$

where ρ_i represents the density of species i, and X_i is the number of particles for species i and X_{total} is the total number of particles. The density of mixtures used in this simulation is referred to as 'Thermodynamics Properties of Chemical and Hydrocarbon' book (Yaws, 2008).

The different types of amine used were 2EAE (2-Ethylamino ethanol), 2DMAE (2-Dimethylamino ethanol) & PZ (Piperazine) with different physical and chemical properties. Analysis of amines was done for 30 wt%, 313 K and 1 atm. Generally 30 wt. % of MEA is used in the gas absorption process due to its fast reaction rate, reasonable absorption capacity, and low cost (Hagewiesche et al., 1995; Ramachandran et al., 2006). MEA is regarded as a benchmark molecule for the CO_2 capture plant (Rochelle, 2009), so analysis of amines in the present study was also done at 30 wt. % and 313 K.

4. Results & discussion

Radial distribution function (RDF) analysis is used to check the intermolecular interaction between amines, CO_2, and water molecules. RDF radial distribution function is a graphical representation of the relationship between r and g(r). Here 'r' is a distance of molecules to neighboring atoms, and g(r) shows the tendency of different atoms to interact with other atoms. Strong intermolecular interaction between atoms will be observed if a higher value of g(r) is obtained at a smaller distance of 'r'. The higher intermolecular interaction will facilitate the absorption process (Harun and Masiren, 2017; Masiren et al., 2016b).

To do the RDF analysis, we need to consider all the bonds involving N, C, H, and O atoms, and Eq. (10) was used to calculate the RDF values for different atoms (Masiren et al., 2016c).

$$gxy(r) = < N_y(r, r + dr)/\rho_y 4\pi r^2 dr \tag{10}$$

Where $N_y(r, r + dr)$ represents the number of atoms in y shells having width Δr at distance r and 'r' represents spherical radius, ρ_y denotes y atom's density, and 'x' indicates the reference atom.

The input model for the production phase is presented in Fig. 1. This model was developed in the amorphous cell module in the MS software (2017) package. It contains 2-ethylamino ethanol, piperazine CO_2 and H_2O. The model in the present study is well in line with the study conducted by (Narimani et al., 2017) on molecular dynamics combines with quantum mechanics for tertiary amines. Although in similar studies of CO_2 absorption into aqueous amine solutions, the COMPASS force field was applied and its validity was confirmed (Narimani et al., 2017; Masiren et al., 2014, 2016a; Maiti et al., 2011; Harun and Masiren, 2017), the simulation results in the present study were validated by comparing the results of previous studies for secondary and tertiary amines with similar methodologies for CO_2 absorption process (Harun and Masiren, 2017; Masiren et al., 2014, 2016a; Harun, 2017; Masiren et al., 2016b).

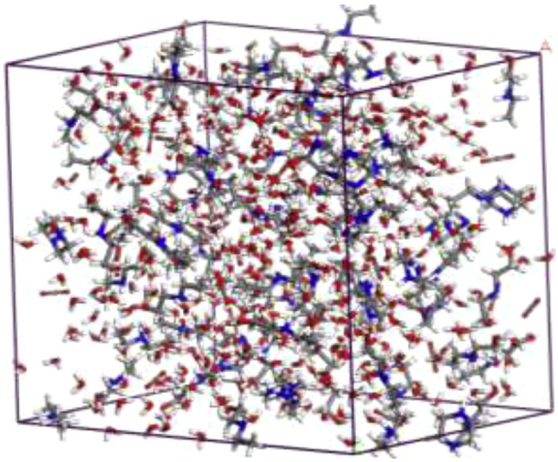

Fig. 1. The amorphous cell structure of aqueous amine solution in Material Studio.

The purpose of the present study is to explore the intermolecular interaction of selected solvent molecules with CO_2. This manuscript includes two types of case studies, first: aim to determine the best amine that has strong intermolecular interaction with CO_2 and water. Second: to explore the effect of piperazine in selected solvents. RDF analysis will be done for four types of solvents, i.e. 2EAE/PZ, pure 2EAE, 2DMAE/PZ & pure 2DMAE.

4.1. Intermolecular interaction of 2EAE and 2EAE/PZ system with water and CO_2

Table 3 shows the summary data of RDF results for pure 2EAE and blended 2EAE/PZ system. Radial distribution function analysis was used to study the intermolecular interaction between amines, CO_2 and water. It gives the relationship between 'r' and g(r) by graphical representation. The peak value in a graphical representation of RDF indicates the highest tendency to interact for that particular interaction. It is assumed that the interactions after 15A°were neglected. Particular observed interactions are given below

While observing the intermolecular interaction in different amines, it's worth mentioning that the hydroxyl group in amines is responsible for the solubility of amines in water, whereas the amino group gives detail about the reaction with an acidic gas (Kohl and Nielsen, 1997). In the case of pure 2EAE for amino group in water N_{2EAE}-H_{water} we observe the peak at (4.75, 1.08). It means at a distance of 4.75A° the intermolecular tendency g(r) to occur for ammonium group (N_{2EAE}- H_{water}) is 1.08, but in case of blended 2EAE/PZ, the highest tendency for ammonium group interaction is (4.75, 1.27) as shown in Fig. 2. It means at the same distance of 4.75A°, 2EAE/PZ has a higher (17.60 % increment) tendency to interact with water as compared to pure 2EAE. The presence of PZ enhanced the interaction of N_{2EAE} with water.

In the case of hydroxyl group HO_{2EAE}-O_{water} we observe peaks at different distances. While observing pure 2EAE at the distance of 2.25, the tendency to interact is 1.32, but in 2EAE/PZ system at a distance of 3.25, the tendency is 1.69, as shown in Fig. 2. It shows that in the blended 2EAE/PZ system the tendency for intermolecular interaction for the hydroxyl group in water to occur is increased. Pure 2EAE shows weak intermolecular interaction with water. This can be due to the fact that 2EAE is a secondary amine that is more nucleophilic as compared to primary and tertiary amine (Masiren et al., 2016b). These results can be justified by the other studies such as (Masiren et al., 2016b; Harun, 2017) who reported the similar results while comparing the pure

Table 3
Summary Data of RDF Results for 2EAE & Blended 2EAE/PZ System.

	N_{2EAE}-H_{water}	HO_{2EAE}-O_{water}	O_{2EAE}-C_{co2}	N_{2EAE}-C_{co2}	N_{PZ}-H_{water}	N_{PZ}-C_{co2}
2EAE	4.75,1.08	2.25,1.32	5.25,1.19	5.25,1.41	–	–
2EAE/PZ	4.75,1.27	3.25,1.69	4.75,1.30	5.25,1.43	4.75,1.07	4.75,1.20

Note: Author's Formulations and Tabulations.
N_{PZ}; Nitrogen in Pipearzine; **N_{2EAE}** ;Nitrogen in 2EAE; **HO_{2EAE}**; Hydrogen at Oxygen in 2EAE ; **H_{WATER}** ; Hydrogen in water **O_{2EAE}**; Oxygen in 2EAE **C_{CO2}** ; Carbon in CO_2.

secondary amine DEA with tertiary and hindered amines, secondary amine (DEA) shows weak intermolecular interaction as compared to tertiary and hindered amines. Moreover, the secondary amine is regarded as a medium amine in CO_2 absorption efficiency and poses a medium energy requirement for regeneration.

Based on the RDF result for hydroxyl group (O_{2EAE}-C_{CO2}) and amino group (N_{2EAE}-C_{CO2}) with CO_2, the tendency to interact for secondary amines is higher for blended 2EAE/PZ system than pure 2EAE system (Fig.3). In case of pure 2EAE, the highest tendency for hydroxyl group (O_{2EAE}-C_{CO2}) to occur was observed at (5.25, 1.19) whereas, in blended system of 2EAE/PZ, for hydroxyl group (O_{2EAE}-C_{CO2}) the RDF plot gives peak at 1.30 at the distance of 4.75A˚(4.75, 1.30) as shown in Fig. 3. It indicates a 9.24 % increment in intermolecular interaction tendency in a blended 2EAE/PZ system. A similar situation was observed in the case of the amino group (N_{2EAE}-C_{CO2}) with CO_2, 1.42 % increment (5.25, 1.43) in intermolecular interaction tendency in blended 2EAE/PZ rather than pure 2EAE (5.25,1.41) as shown in Fig. 3. Pure 2EAE does not contain N_{PZ}-H_{water} and N_{PZ}-C_{CO2} so that we can neglect them (Fig. 4).

The higher intermolecular interaction results in 2EAE/PZ system can be justified and supported by following reasons; first, the presence of piperazine, as piperazine has two nitrogen atoms in its molecular structure, which increase the absorption of CO_2. Moreover, the cyclic structure of piperazine may favor the rapid formation of carbamates (Cullinane and Rochelle, 2004). It is also stated that PZ has a higher absorption capacity and widely used as a rate promoter (Bishnoi and Rochelle, 2000). The rate constant of PZ is much higher than conventional alkanol amine like MEA (Idem et al., 2009). Second, the secondary amine 2EAE; in previous studies, it is reported that secondary amines have a lower enthalpy of desorption than primary amines. This is due to the unstable or weak formation of carbamates while reacting to the secondary amines with CO_2. Therefore less energy is required in the desorption process of secondary amines as compared to primary amines (Hwang et al., 2017). Furthermore, 2EAE has fast reaction kinetics as compared to other secondary amines (like 2MAE or 2BAE), and reaction kinetics of 2EAE is close to MEA (El Hadri et al., 2017). As a result, 2EAE shows higher intermolecular interaction in 2EAE/PZ blend.

The results show that in all types of interaction, the blend of 2EAE/PZ has higher intermolecular interaction with CO_2 and water, thus a higher tendency to interact with CO_2 in 2EAE/PZ rather than pure 2EAE. Moreover, the addition of piperazine increased the intermolecular interaction in 2EAE and facilitated the absorption process. There is significant increase in all types of the intermolecular interactions in the presence of PZ except N_{2EAE}-C_{CO2}. The intermolecular interaction of N_{2EAE}-C_{CO2} in 2EAE system is 1.41, whereas the interaction in 2EAE/PZ system is 1.43 at a distance of 5.25. Although, the presence of piperazine also increased the intermolecular interaction of N_{2EAE}-C_{CO2} in 2EAE system but, the effect is weak. The blended 2EAE/PZ can be a good choice for CO_2 absorption. Although the interaction of blended 2EAE/PZ is higher than pure 2EAE, but the interaction of pure 2EAE with CO_2 is also important and cannot be neglected as there is no huge difference in intermolecular interaction of pure and blended 2EAE. According to experimental studies, 2EAE has higher loading (mol CO_2 /mol amine) (0.71) than MEA (0.58), and absorption heat of 2EAE (68.59 kJ/mol) is lower than that of MEA (85.13 kJ/mol). Moreover, the kinetics and thermodynamic studies show that it can be an alternative to benchmark molecule as MEA, which is used in conventional CO_2 capture processes (El Hadri et al., 2017; Ahmad et al., 2018). So 2EAE can be suggested for further studies for CO_2 absorption.

4.2. Intermolecular interaction of DMAE & blended DMAE/PZ with CO_2 and water

Table 4 shows the summary of results for intermolecular interaction in pure DMAE and blended DMAE/PZ with CO_2 and water. In the case of pure DMAE for amino group N_{DMAE}-H_{water} in water, the peak of intermolecular interaction tendency was observed at (4.75, 1.25), as shown in Fig. 5. Whereas, for blended DMAE/PZ, the tendency g(r) to occur at the distance of 1.28 is 4.75Aº (4.75, 1.28) (Fig. 5). It indicates that at the same distance of 4.75A˚, the tendency for amino group N_{DMAE}-H_{water} in water for blended DMAE/PZ is 2.4 % higher than that of pure DMAE. The same situation is observed in the hydroxyl group

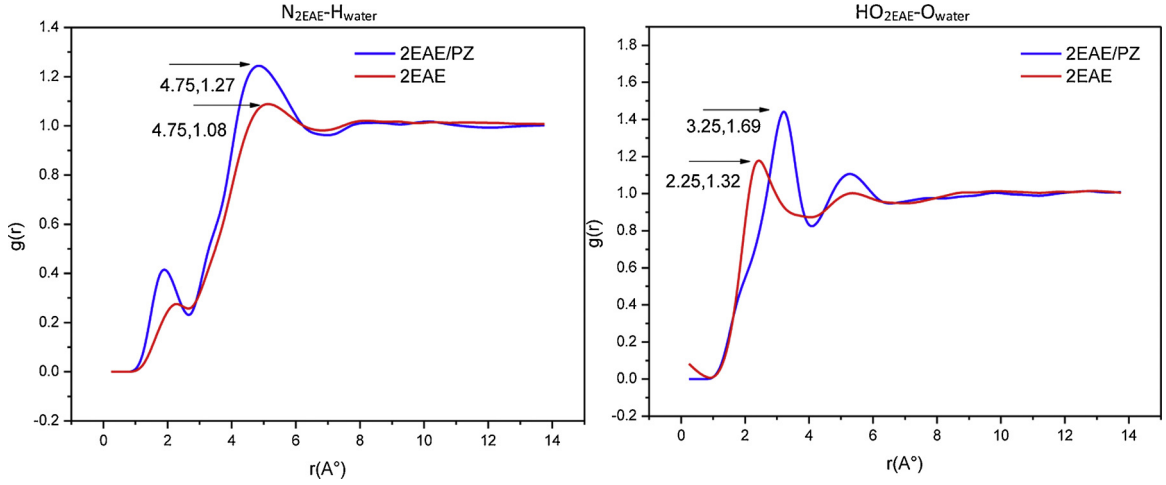

Fig. 2. Intermolecular interactions of 2EAE/PZ and 2EAE with water.

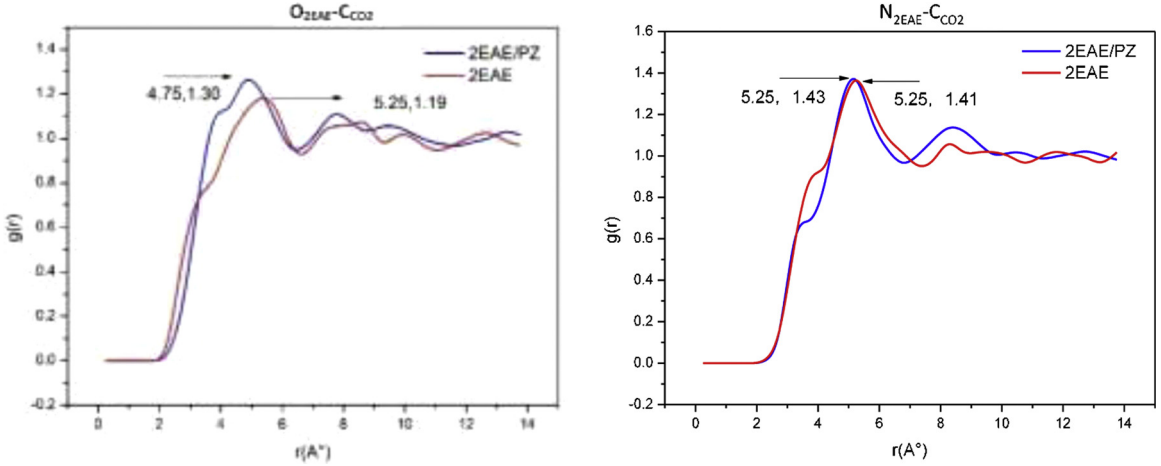

Fig. 3. Intermolecular interactions of 2EAE/PZ and 2EAE with CO_2.

HO_{DMAE}-C_{CO2}. There is a 7.6 % increment in intermolecular tendency to occur in a blended DMAE/PZ system than in pure DMAE system. It means pure DMAE cannot easily form hydrogen bond in water but DMAE with PZ can easily make hydrogen bond in water.

The interaction of DMAE and blended DMAE/PZ with CO_2 shows that in case of hydroxyl group with CO_2 (O_{DMAE}-C_{CO2}), the interaction tendency to occur is higher (3.6 % increment) in blended DMAE/PZ system (5.25, 1.15) than pure DMAE (5.25, 1.11) as shown in Fig. 6. At the same distance of 5.25A°, the tendency for hydroxyl group with CO_2 to occur is 1.15 in the blended DMAE/PZ system, but in pure DMAE system, it is noted to be 1.11. A similar situation is observed in the amino group with CO_2 (N_{DMAE}-C_{CO2}); the tendency in blended DMAE/PZ is higher than pure DMAE system (2.2 % increment) in blended DMAE/PZ as compare to pure DMAE (Fig. 6).

It can be elaborated that DMAE with PZ has a higher tendency to interact with CO_2, and the hydroxyl (O_{DMAE}-C_{CO2}) and amino group (N_{DMAE}-C_{CO2}) are more attractive to CO_2 in blended DMAE/PZ system. These results are in line with previous studies such as (Harun and Masiren, 2017) reported while comparing pure MDEA and MDEA/PZ, MDEA/PZ shows higher intermolecular interaction tendency than pure MDEA. The higher intermolecular interaction tendency in MDEA/PZ system is due to PZ, as the presence of PZ enhanced the strength of intermolecular interaction in MDEA/PZ. In the present situation, DMAE is also a tertiary amine and does not contain hydrogen atom at the amino group. Due to this fact, it cannot directly react with CO_2. But in the case of blended DMAE/PZ, PZ first reacts with CO_2 and accelerates the reaction (Bishnoi and Rochelle, 2000). As a result, we observe higher intermolecular interaction in blended DMAE/PZ than pure DMAE.

Experimental studies of primary, secondary, and tertiary amines show that the order for selectivity of these amines towards CO_2 is as primary amine > secondary amine > tertiary amines (Ciftja et al., 2013). It elaborates that the tertiary amines are less attractive to CO_2 as compared to primary and secondary amines. Therefore in the present scenario, the order of intermolecular interaction in DMAE/PZ and pure DMAE is DMAE < DMAE/PZ. Another reason for low intermolecular interaction in DMAE is that it contains two methyl groups and one ethanol group at the nitrogen atom. It is reported that the addition of methyl and alcohol substitution at the nitrogen atom decreases the amine reactivity with CO_2 (Idris and Eimer, 2014). Pure DMAE does not contain N_{PZ}-C_{CO2} and N_{PZ}-H_{Water}, so we can neglect it (Fig. 7).

In the present study, it is observed that both the secondary and tertiary blends with piperazine show higher intermolecular interaction tendency towards CO_2 as compared to pure secondary and a tertiary amine. Furthermore, PZ is proved as a rate promoter as it increased the intermolecular interaction in both types (secondary and tertiary) of the blend. Higher intermolecular interaction in any blended or pure amine means it can facilitate the absorption process and may lead to an

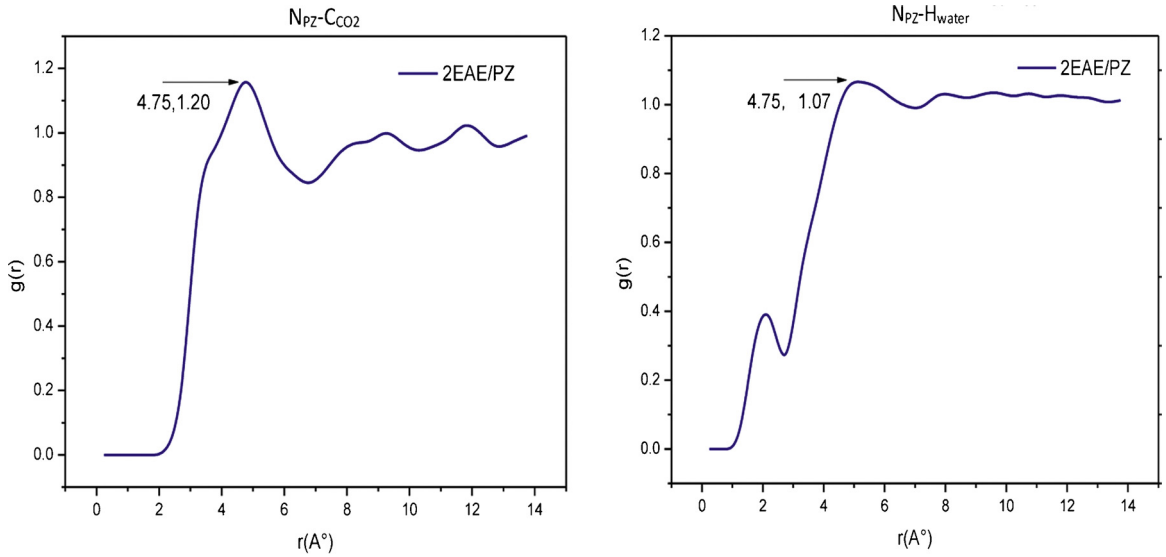

Fig. 4. Intermolecular interaction of 2EAE/PZ with CO_2 and H_2O.

Table 4
Summary of RDF results for DMAE & blended DMAE/PZ system.

Particulars	N_{DMAE}-H_{water}	HO_{DMAE} O_{water}	O_{DMAE}-C_{CO2}	N_{DMAE}-C_{CO2}	N_{PZ}-H_{water}	N_{PZ}-C_{CO2}
DMAE	4.75,1.25	3.25,1.31	5.25,1.11	5.25,1.75	–	–
DMAE/PZ	4.75,1.28	3.25,1.41	5.25,1.15	5.25,1.79	5.25,0.97	5.75,1.41

Note: Author's Formulations and Tabulations.
N_{DMAE}; Nitrogen in Dimethylamino ethanol **N_{PZ}**; Nitrogen in Pipearzine; **HO_{DMAE}**; Hydrogen at Oxygen in DMAE; **H_{WATER}**; Hydrogen in water **O_{DMAE}**; Oxygen in DMAE; **C_{CO2}** ; Carbon in CO_2.

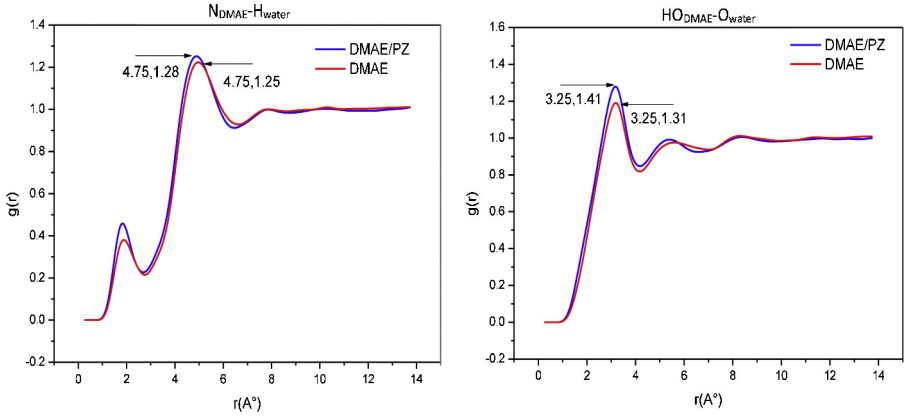

Fig. 5. Intermolecular interactions of DMAE/PZ and DMAE with water.

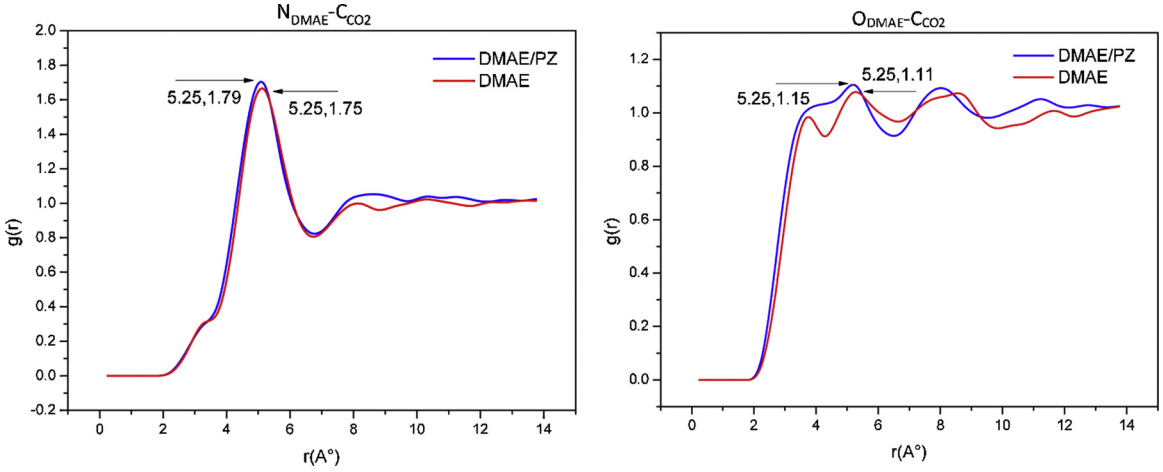

Fig. 6. Intermolecular interactions of DMAE/PZ and DMAE with CO_2.

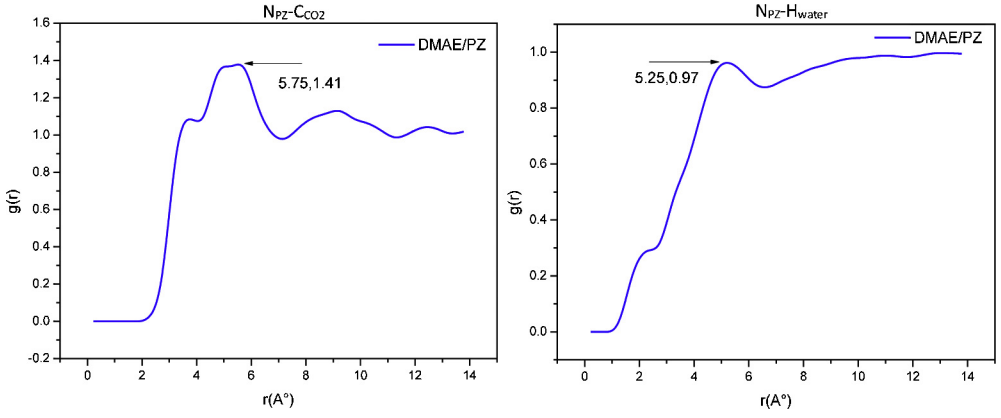

Fig. 7. Intermolecular interaction of 2DMAE/PZ with CO_2 and H_2O.

increase in the rate of absorption for CO_2 capture process.

The findings of present study indicate that 2EAE and 2DMAE mixed with PZ show a strong intermolecular interaction with CO2. These results can be compared with the findings of existing experimental studies such as; (El Hadri et al., 2017, El Hadri et al., 2015, Liu et al., 2019; Ahmad et al., 2018; Hwang et al., 2017). The results of these studies indicated that 2EAE and 2DMAE have good CO2 absorption, low heat of absorption and high energy efficiency for CO2 removal. Thus, comparing the results in the present study and the findings in existing literature, it is concluded that the 2EAE and 2DMAE can be suggested as potential absorbents for industrial application for CO2. Moreover, the agreement between the results of simulation and experimental data confirms the simulation methodology and suitability of forcefield used in present study.

5. Conclusion

The influence of 2EAE, 2DMAE, and PZ in the application of the CO_2 absorption process through a molecular point of view is investigated. Four different types of aqueous solvent systems were studied, i.e., 2EAE/PZ, 2DMAE/PZ, pure 2EAE, and pure 2DMAE (DMAE). The molecular dynamic simulation study was used to check the physical interaction between different atoms so that the solvent system with higher intermolecular interaction can be selected for experimental studies. Radial distribution function analysis was used to check the intermolecular interaction between amines and CO_2. The results obtained were as follows,

(1) In comparison to pure 2EAE and blended 2EAE/PZ system, the blended system shows stronger intermolecular interaction in all types of discussed bonds. It indicates that 2EAE/PZ have a higher tendency to interact with CO_2 as PZ helps to increase the reaction rate. The higher intermolecular interaction illustrates that the blend of 2EAE + PZ is more reactive to CO_2 and can increase the absorption process, which may help to increase the reaction kinetics, which helps in the reduction of solvent circulation rate in capture plant. In this way, this study can help to select a solvent with a higher absorption rate to reduce the circulation rate of absorbent and thus to reduce the equipment size in the capture plant.

(2) While comparing the pure DMAE and blended DMAE/PZ, it was observed that blended amines DMAE/PZ shows a higher tendency to interact with CO_2 than pure DMAE. The overall reaction rate in tertiary amines is slower as compared to secondary amines. Thus the higher intermolecular interaction in DMAE/PZ is due to the presence of PZ. So in both of these case studies, it is obvious that the small addition of PZ to the solvent system increases the intermolecular interaction in 2EAE/PZ and DMAE/PZ.

CRediT authorship contribution statement

Maimoona Sharif: Conceptualization, Methodology, Software. **Tingting Zhang:** Writing - review & editing. **Xiaomei Wu:** Visualization, Investigation. **Yunsong Yu:** Validation, Visualization. **Zaoxiao Zhang:** Supervision, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.ijggc.2020.103059.

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