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Structure and activity relationships for amine-based CO_2 absorbents-II

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A B S T R A C T

A study to determine the structure and activity relationships of various amine-based CO_2 absorbents was performed, in which the absorption of pure CO_2 at atmospheric pressure was measured to assess the total absorption rates and capacities. Steric hindrance effect was noticed when side chain with alkyl group was present at the α-carbon to the amine group in the absorbent structure. An increase in the number of amine groups in absorbent structure, results in a higher capacity of upto 3.03 moles CO_2/moles amine. Aromatic amines substituted with alkyl groups at the 2nd and 5th position show an increase in both absorption rate and capacity.

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Keywords: CO_2; Amine; Absorption; Acid gas

1. Introduction

Although the absorption of acid gases such as CO_2 in aqueous amine solutions like e.g. MEA (monoethanolamine) from natural gas concerns proven technology, the removal of CO_2 from flue gases is not as straightforward as expected. In these oxygen-containing systems problems such as degradation, precipitation, corrosion, foaming, etc., affect the process. Furthermore, in the currently used systems a major part of the operational costs is caused by the solvent regeneration (up to 40%). Therefore, a need exists to develop novel solvent systems for the removal of carbon dioxide from flue gases.

Clearly, relationships exist between the amine structure and the activity and capacity for CO_2 absorption. According to Chakraborty et al. (1986) the introduction of substituents at the α-carbon creates a carbamate instability, which causes the hydrolysis to go faster, thus increasing the amount of bicarbonate, allowing for higher CO_2 loadings. Sartori and Savage (1983) suggested this instability was due to the steric hindrance created by these α-substituents. Chakraborty et al. (1988) examined the electronic effects of such substituents and proposed that substitution at the carbon atom results in an interaction of the π and π^* methyl group orbital with the lone pair of the nitrogen. This interaction reduces the charge at the nitrogen, resulting in a softer base, which again results in a weakening of the N–H bond. These effects allow an increase of the hydrolysis by the hydroxide (hard base) in the solution. The steric hindrance would be expected to slow the rate of the initial reaction with CO_2 to some extent, but as 1 mol of amine is released upon hydrolysis of the carbamate, the level of amine available for reaction with CO_2 increases.

To obtain a better understanding of the structure–activity relationship, solvent screening experiments were performed. The variables that were investigated were, e.g., the chain length, an increase in the number of functional groups, the presence of a side chain at the α-carbon position, the alkyl group position in cyclic amines and side chain effects on cyclic amines with different functional groups, etc. A semi-quantitative representation of these effects on the initial rate of absorption for CO_2 is described, as well as the capacity of various solvents for CO_2 absorption.

2. Experiment

The various amine-based absorbents were tested in a screening apparatus (procedure as described by detail in article Singh et al., 2007) where relative rates of absorption and absorption capacity can be measured and compared to the MEA default

case. Most of the absorbents tested have a good solubility in water. However, some amine-based absorbents concentration in the solution could vary with the type of compound only to, e.g. molecular weight and solubility. This implies that the molar concentrations for the absorbents used in these experiments are not the same in some cases, e.g. hexylamine, triethylenepentamine. As a default case MEA was chosen with a concentration of 2.5 mol/l. An absorption time of 200 min was found to be suitable for most of the compounds to reach the equilibrium.

In this paper the main focus is still on the behaviour of the different chemical species and their reactive properties for CO_2 absorption. The optimal operational concentrations for these absorbents are not yet known a priori, so a comparison based on molar concentration might be as good as one based on weight fraction. Hence, both type of comparison for the amine-based absorbents are discussed in these results. All chemicals investigated (see Tables 1–10) were purchased from Sigma–Aldrich Chemical Co.

3. Results and discussion

Examination of the absorption from a pure CO_2 atmosphere, where saturation was reached for basically all absorbents within the experimental time frame, allows for a comparison of the absorption rates and saturation values. From the initial absorption rates an indication can be obtained about the reactivity of various amine-based absorbents. It must be noticed, however, that due to the mass transfer effects, e.g. interfacial area and enhancement factor, that are contactor specific, no quantitative conclusions can be presented. However, the stirring speed was the same for the al absorbents so, differences would arise mainly due to variations in interfacial tension, density, viscosity and heat of absorption, which are characteristics for each compound.

3.1. Effect of side chain

The position of different functional groups in the structure of various amine-based absorbents is an important factor. In Figs. 1–3 and Table 1 the effect of the position of substituted hydroxyl groups is compared. It should be noticed that the concentration for 3-amino-1-propanol, and 2-amino-1-butanol was kept at 2.5 mol/l, whereas concentration used
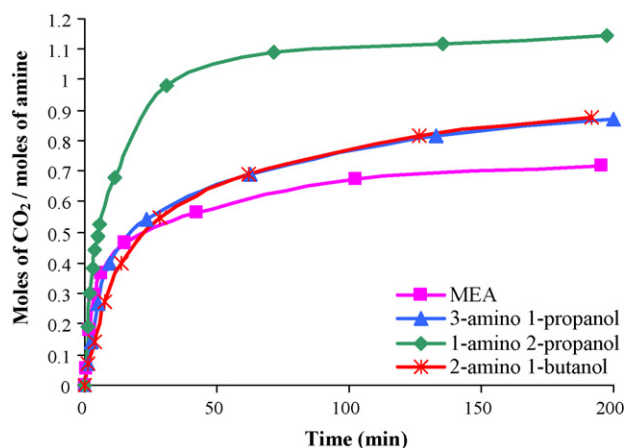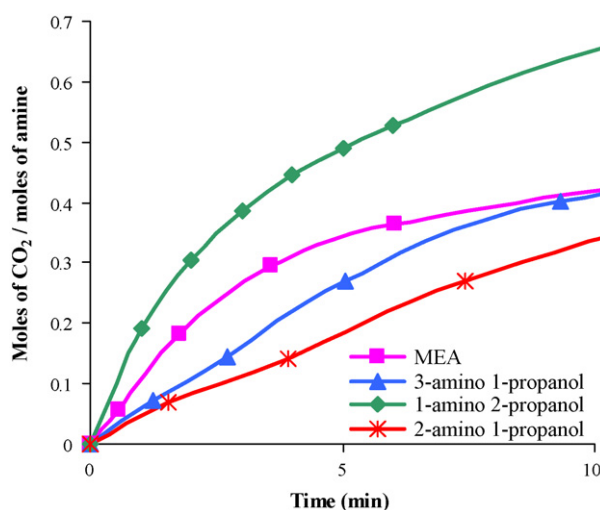

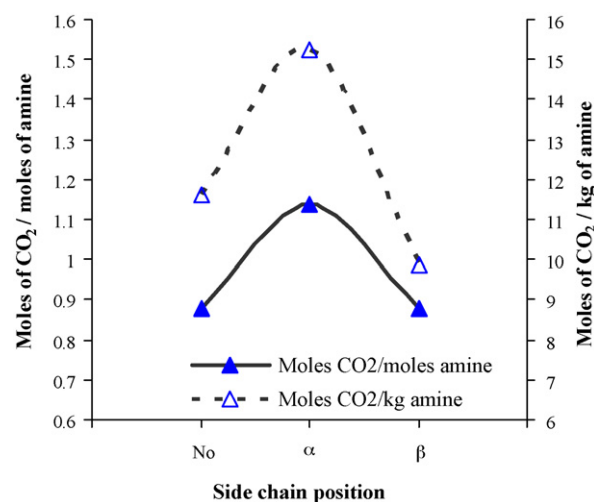Fig. 2 – Influence of a hydroxyl group substitution for the absorption of CO_2 in aqueous absorbents.

Fig. 3 – Influence of a hydroxyl group substitution on total loading for CO_2 absorption.

for 1-amino-2-propanol was 0.5 mol/l. In these experiments the hydroxyl group is positioned at the α-carbon (2-amino-1-butanol) and β-carbon (1-amino-2-propanol) to the amine group in the absorbent structure. The concentration of all alka-

Fig. 1 – Influence of the OH group position in the substituted alkanolamine for the absorption of CO_2 in aqueous absorbents.

Table 1 – Total capacity of aqueous alkanolamine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)

Aqueous absorbent	CO$_2$ loading	
	A	B
H$_2$N⌒OH 3-Amino-1-propanol	0.88	11.63
H$_3$C⌒NH$_2$ OH 1-Amino-2-propanol	1.14	15.24
OH H$_3$C⌒NH$_2$ 2-Amino-1-butanol	0.88	9.86

nolamine absorbents was kept 2.5 mol/l. In Fig. 1 the overall results are presented. It must be noticed that a substitution of an OH group on the α-carbon (2-amino-1-butanol) to the amine group increased the total absorption capacity upto 1.14 moles CO_2/moles amine when compared with an OH group substitution on the β-carbon (1-amino-2-propanol) 0.88 moles CO_2/moles amine (see Table 1). It is clear from these values that the amine-based absorbent substituted with a hydroxyl group at α-carbon (2-amino-1-butanol) to the amine group results in an increase in absorption capacity. This result clearly shows the effect of steric hindrance caused by hydroxyl group substitution at the amine group (Chakraborty et al., 1986, 1988; Hook, 1997).

Fig. 2 shows the effect of a hydroxyl group substitution on α-carbon (1-amino-2-propanol) to the amine group results in an increase in the initial absorption rate when compared with a OH group substitution on the β-carbon (2-amino-1-butanol). At this stage no further qualitative analysis will be presented on the initial absorption rate, as the absorption rate is a complex interaction between mass transfer, kinetics and equilibrium. The interpretation is not as straightforward as was expected before hand. Comparing the total absorption capacities in unit moles of CO_2/kg of amine showed in (see Fig. 3) results showed an increase in the absorption capacity for a hydroxyl group substitution on the α-carbon (1-amino-2-propanol) to the amine group as well.

Furthermore, the effect of a methyl group substitution at the α or β carbon to the amine group in alkylamines was investigated (see Figs. 4–6 and Table 2). The concentration of butylamine, sec-butylamine and isobutylamine used in the experiment was 2.5 mol/l. Fig. 4 shows the overall results from these substituted alkyl absorbents. Substitution of the CH_3 group at the α-carbon (sec-butylamine) to the amine group increased the absorption capacity upto 0.84 moles CO_2/moles amine when compared with a CH_3 group substitution on the β carbon to the amine group (isobutylamine 0.78 moles CO_2/moles amine) (see Table 2). This might be due to the fact that the substitution at the α-carbon position creates steric hindrance effect and thus lowers the stability of carbamate. This means that the hydrolysis of the carbamate is enhanced which will drive the equilibrium to the bicarbonate.

Fig. 5 shows the effect of an alkyl group substitution on the initial absorption rate. The results shows that the alkyl group substitution on the α-carbon (sec-butylamine) to the amine group decreased the initial absorption rate when com-
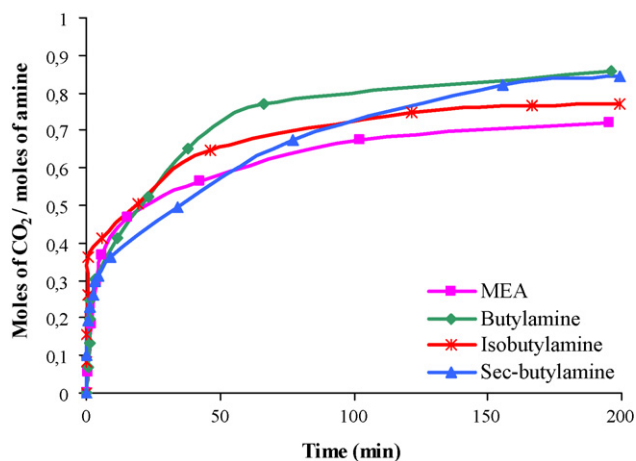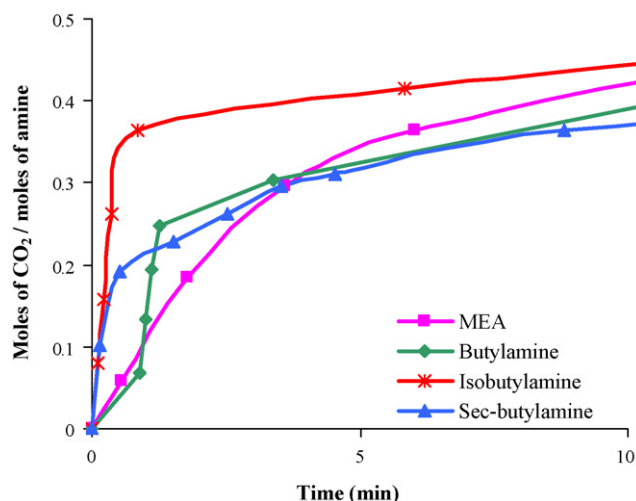

Fig. 5 – Influence of a methyl group substitution for the absorption of CO_2 in aqueous absorbents.

pared to a substitution on the β-carbon to the amine group (iso-butylamine). The decrease in initial absorption rate in sec-butylamine might be caused by the effect of steric hinderance at the amine group, which decreased the initial absorption rate.
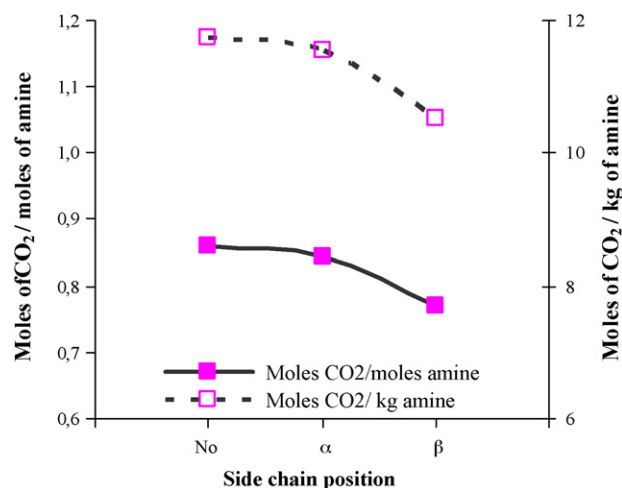

Fig. 6 – Influence of a methyl group substitution on total loading for CO_2 absorption.

Fig. 4 – Influence of a methyl group substitution in the structure for the absorption of CO_2 in aqueous absorbents.

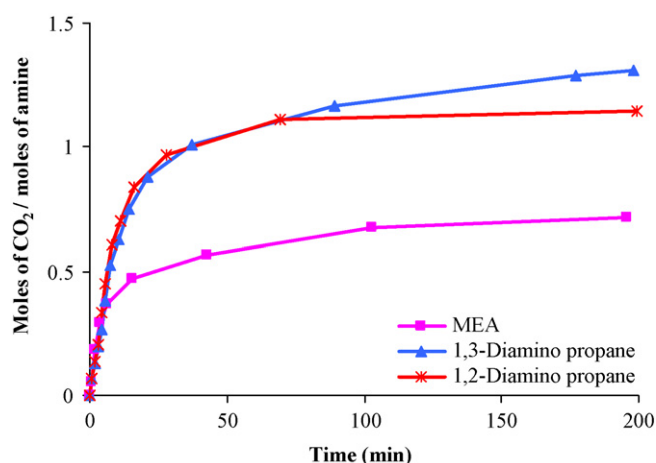| Table 2 – Total capacity of aqueous amine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)		
Aqueous absorbent	CO$_2$ loading	
	A	B
Butylamine	0.86	11.74
Sec-butylamine	0.84	11.54
Isobutylamine	0.78	10.54

Fig. 7 – Influence of the amine group position in diamines for the absorption of CO_2 in aqueous absorbents.

Similar observations of the adverse effect of steric hindrance on amine-CO_2 absorption rates have been made previously (Sartori and Savage, 1983). Clearly steric hinderance around the amine group reduces the initial rate of reaction, even though in time these hindered amines absorb more carbon dioxide.

The influence of an amine group substitution by a side chain in diamines was also investigated. Fig. 7 shows the overall absorption results. It should be noticed that the concentration of 1,2-diamino propane and 1,3-diamino propane was kept at 2.5 mol/l.

The amine group substitution at the β-carbon to the amine group (1,2-diamino propane) caused a decrease in the absorption capacity (1.27 moles CO_2/moles amine) when compared with the non-substituted (1, 3-diamino propane) (1.30 moles CO_2/moles amine (see Table 3)).

The results from Figs. 7 and 8 shows that there was a slight decrease in the initial absorption rate for an amine group substitution at the β-carbon to the amine group (1, 2-diamino propane) compared to non-substituted diamines such as 1,3-diamino propane. From Fig. 9 and Table 3 it is clear that the absorption capacity decreased slightly from 1.30 to 1.27 moles CO_2/moles amine with a substitution of the amine group. Hence, amine group substitution on the β-carbon to the amine
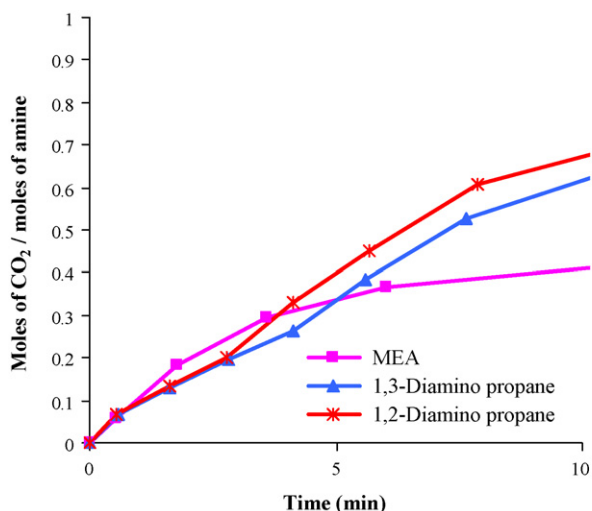

Fig. 8 – Influence of amine group position in diamines for the absorption of CO_2 in aqueous absorbents.
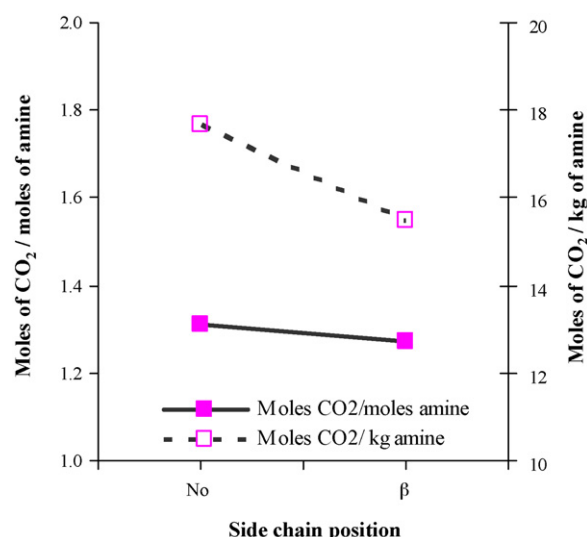

Fig. 9 – Influence of amine group position in diamine total loading for CO_2 absorption.

group in the structure did not show a strong influence on the initial absorption rate and capacity.

3.2. Effect of number of functional groups

The effect of an increase in the number of functional groups was investigated. It should be noticed that the concentration of ethylenediamine, diethylenetriamine and triethylenetetramine was kept at 2.5 mol/l. Due to the high viscosity of tetraethylenepentamine, the concentration used for this absorbent was kept at 0.5 mol/l. In Figs. 10–12 and Table 4, the result from the effect of an increase in number of amine groups in the absorbent structure are presented. The results from Figs. 10 and 11 show that an increase in the number of amine groups from 2 (ethylenediamine) to 3 (diethylenetriamine) resulted in a slight increase in the initial absorption rate, whereas there is a drastic increase in the initial absorption rate when the number of amine group increases up to 4 (trietheylenetetramine). A further increase of the number of amine groups up to 5 (tetraethylenepentamine) did not increase the initial absorption rate.

The effect of an increase in the number of amine groups on the absorption capacity can be seen in Fig. 12 and Table 4. An increase in the number of amine groups increased the capacity from 1.83 to 3.03 moles CO_2/moles amine. This might be caused by the increase in the number of amine groups, which creates more reaction sites available for the reaction

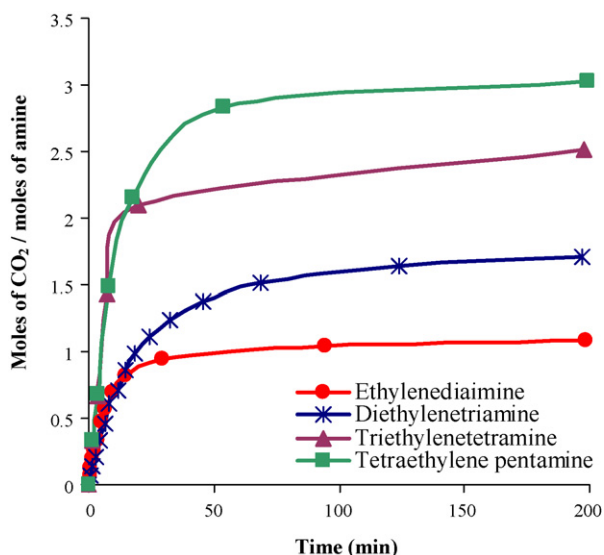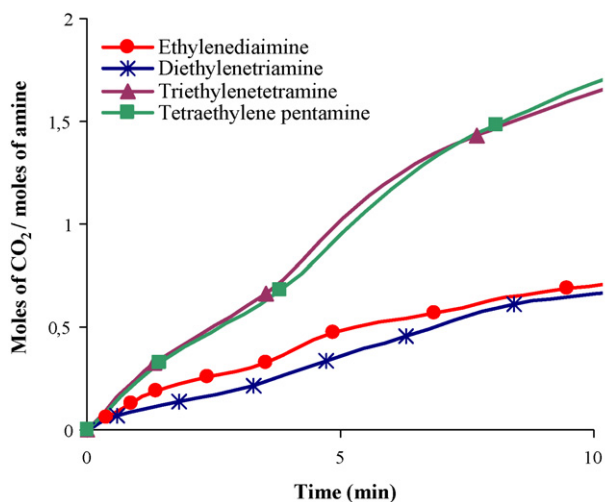| Table 3 – Total capacity of aqueous amine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)		
Aqueous absorbent	CO₂ loading	
	A	B
H_2N NH_2 1,3-Diamino propane	1.30	17.66
H_3C NH_2 NH_2 1,2-Diamino propane	1.27	15.48

Fig. 10 – Influence of the number of amine groups in the absorbent structure for the absorption of CO_2 in aqueous absorbent.

with CO_2. Furthermore when the total absorption capacity of these absorbents was compared in unit of kg of CO_2 absorbed per mole of amine, results show that the absorption capacity did not increase with increase in number of amine group in the structure, for example ethylenediamine (where two amine groups are present) could absorb up to 17.93 kg CO_2/moles amine, whereas tetraethylenepentamine (in which 5 amine groups are present) could absorb up to 15.98 kg CO_2/moles amine (see Table 4).

The effect of an increase in the number of hydroxyl groups was also investigated. The concentration of *N*-(2-hydroxyethyl) ethylenediamine and *N*,*N'*-bis (2-hydroxyethyl) ethylenediamine) was 2.5 mol/l. The results from diamine-based absorbent with one (*N*-(2-hydroxyethyl) ethylenediamine) and two hydroxyl groups (*N*,*N'*-bis(2-hydroxyethyl) ethylenediamine) are presented in Figs. 13–15 and Table 5. Figs. 13 and 14 shows that increasing the number of hydroxyl groups in diamine-based absorbent structures results in a negative effect on the initial absorption rate, resulting in a decrease in the initial absorption rate. This might be caused by the presence of a steric hindrance effect around both amine
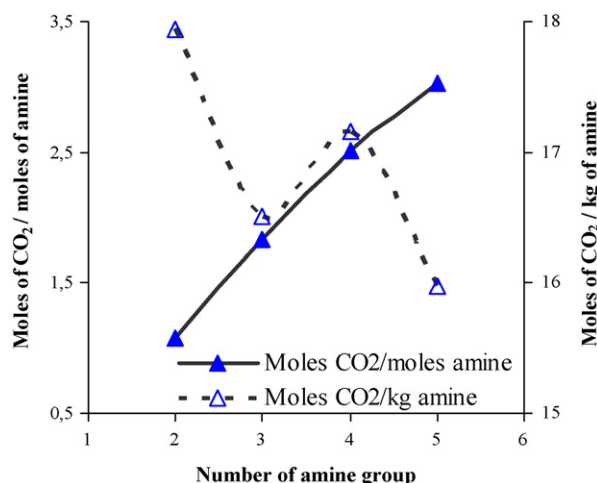

Fig. 12 – Influence of number of amine group position on total loading for CO_2 absorption.

Table 4 – Total capacity of aqueous amine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)

Aqueous absorbent	CO_2 loading	
	A	B
H_2N ~ NH_2 Ethylenediamine	1.08	17.93
H_2N ~ N(H) ~ NH_2 Diethylenetriamine	1.83	16.51
H_2N ~ N(H) ~ N(H) ~ NH_2 Triethylenetetramine	2.51	17.15
H_2N ~ N(H) ~ N(H) ~ N(H) ~ NH_2 Tetraethylenepentamine	3.03	15.98

Fig. 11 – Influence of number of amine group position for the absorption of CO_2 in aqueous absorbents.
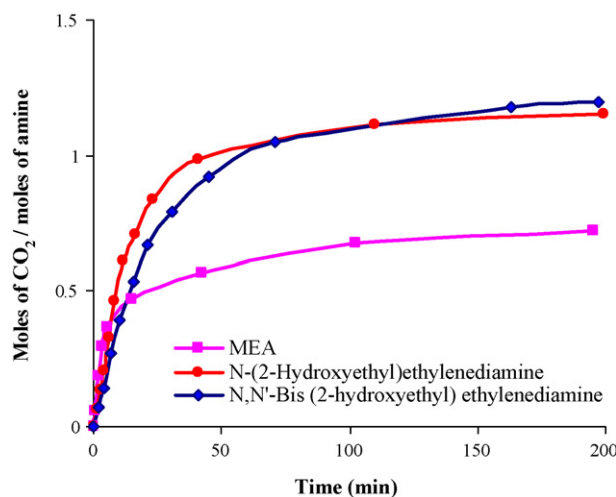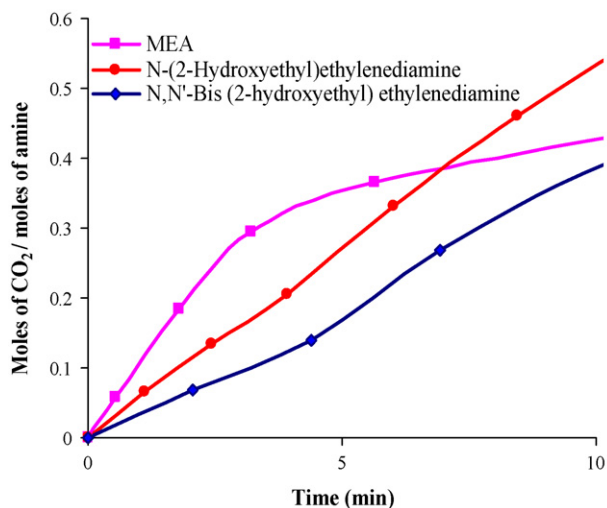

Fig. 13 – Influence of the number of OH group in the structure for the absorption of CO_2 in 2.5 M aqueous absorbents.

Fig. 14 – Influence of number of amine group position for the absorption of CO_2 in aqueous absorbents.
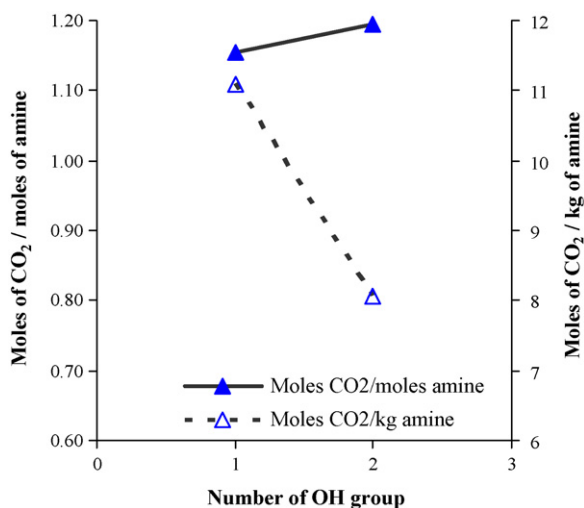

Fig. 15 – Influence of number of amine group position on total loading for CO_2 absorption.

groups when two hydroxyl groups are present (N,N'-bis(2-hydroxyethyl) ethylenediamine).

From Fig. 15 and Table 5 it is clear that an increase in the number of hydroxyl groups in the absorbent structure increased the absorption capacity somewhat from 1.15 to 1.20 moles CO_2/moles amine. This result indicates the steric hindrance effect caused by an increase in the number of hydroxyl groups in amine-based absorbent structure.

Table 5 – Total capacity of aqueous amine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)		
Aqueous absorbent	CO_2 loading	
	A	B
HO⌒⌒⌒NH₂ HN⌒ N-(2-hydroxyethyl) Ethylenediamine	1.15	11.09
HO⌒NH⌒⌒NH⌒OH N,N'-bis(2-hydroxyethyl) Ethylenediamine	1.20	8.07
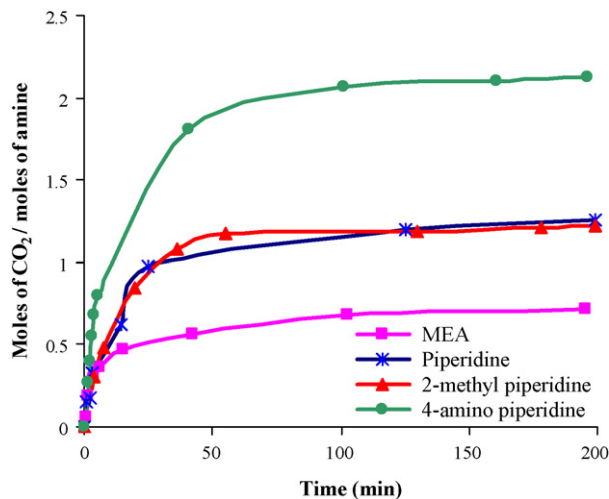
Fig. 16 – Influence of a substitution on saturated cyclic amines for the absorption of CO_2 in aqueous absorbents.

When comparing the absorption capacity in unit of moles of CO_2/kg of amine (see Table 5 and Fig. 15) this shows a decrease in the absorption capacity from 11.09 to 8.07 moles of CO_2/kg of amine with an increase in the number of hydroxyl groups. Therefore, from these results it is clear that increase in the number of hydroxyl groups result in somewhat higher absorption capacities in unit of moles CO_2/moles amine, but decreases the initial absorption rate.

3.3. Effect of functional groups in cyclic amines

Cyclic amines are potential absorbents for CO_2 absorption due to their fast absorption rate and higher absorption capacities. Therefore, the effect of different substituted saturated and unsaturated cyclic amines was investigated. In Figs. 16–18 and Table 6 the comparison between saturated monoamine and similar compounds, substituted with an alkyl and amine groups, is presented. It must be noticed that the concentration of piperidine and 2-methylpiperidine was kept to be 0.5 mol/l, whereas for 4-amino piperidine the concentration was 0.25 mol/l.

Figs. 16 and 17 shows that the substitution with a methyl group at the second position in the saturated ring
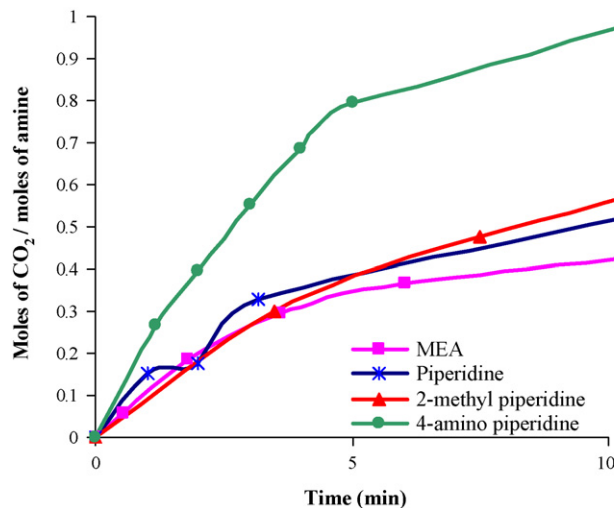

Fig. 17 – Influence of number of alkyl group for the absorption of CO_2 in aqueous absorbents.
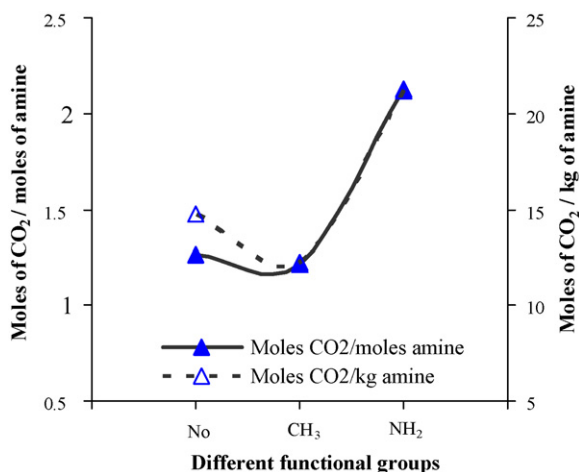
Fig. 18 – Influence of number of alkyl group on total loading for CO_2 absorption.

(2-methyl piperidine) increased the initial absorption rate somewhat whereas substitution of an amine group at the side chain of a saturated ring (4-amino piperidine) substantially increased the initial absorption rate substantially. Clearly an amine group substitution in a saturated cyclic ring increased the protonation reaction, thus increasing the absorption rate.

However, the absorption capacity remained, similar with a substitution of a methyl group in a saturated ring (1.22 moles CO_2/moles amine, see Fig. 18 and Table 6). When piperidine was substituted with an amine by side chain on the saturated cyclic ring, i.e. 4-aminopiperidine, the absorption rate doubled when compared with piperidine, reaching up to 2.12 moles CO_2/moles amine (see Table 6). This might be explained by the fact that in 4-aminopiperidine there are more amine groups, resulting in higher CO_2 absorption capacities.

In Figs. 19–21 and Table 7 the effect of a methyl group substitution on saturated cyclic diamines is shown. The concentration of piperazine, 2-methylpiperazine and *trans*-piperazine, 2,5-dimethyl was 0.5 mol/l. Figs. 18 and 19 shows that a substitution of one methyl group in the saturated ring at the 2nd carbon position increased the initial absorption rate when compared with two methyl group substitutions on the 2nd and 5th position in the saturated ring. This might
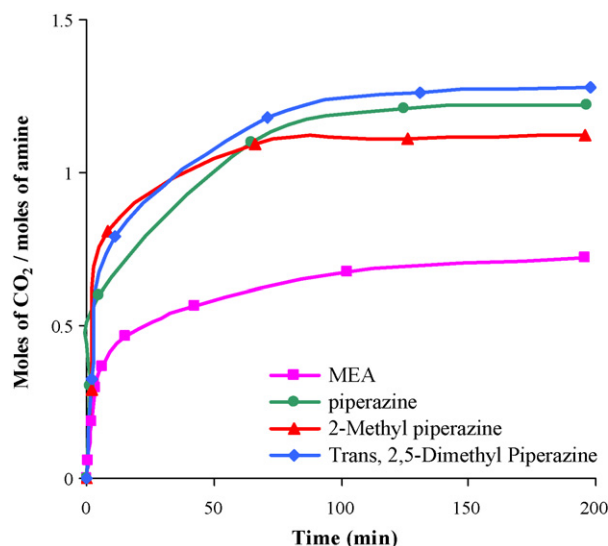
Fig. 19 – Influence of a methyl group substitution on saturated cyclic diamine for the absorption of CO_2 in aqueous absorbents.

be caused by the fact that in aromatic amines, substitution with a functional group at the 2nd and/or at the 5th position increases the basicity of the compounds. Increasing the basicity will allow for a faster protonation of the amine group thus
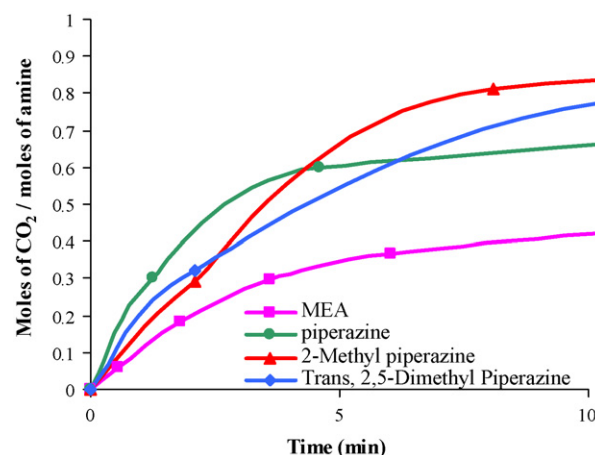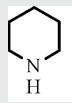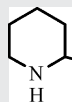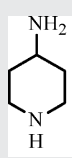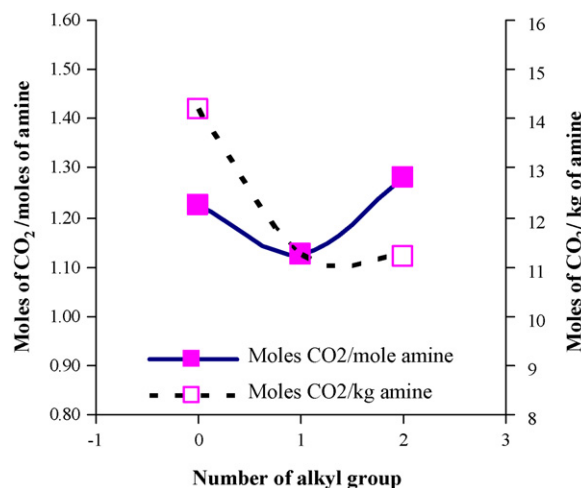

Fig. 20 – Influence of number of alkyl group for the absorption of CO_2 in aqueous absorbents.

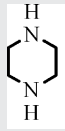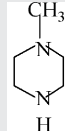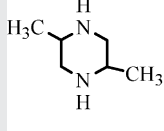| Table 6 – Total capacity of aqueous amine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)		
Aqueous absorbent	CO_2 loading	
	A	B
Piperidine	1.26	14.79
2-Methylpiperidine	1.22	12.28
4-Aminopiperidine	2.12	21.20

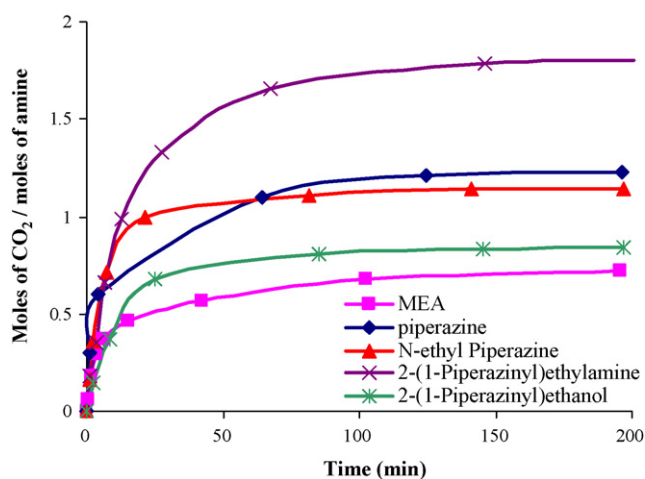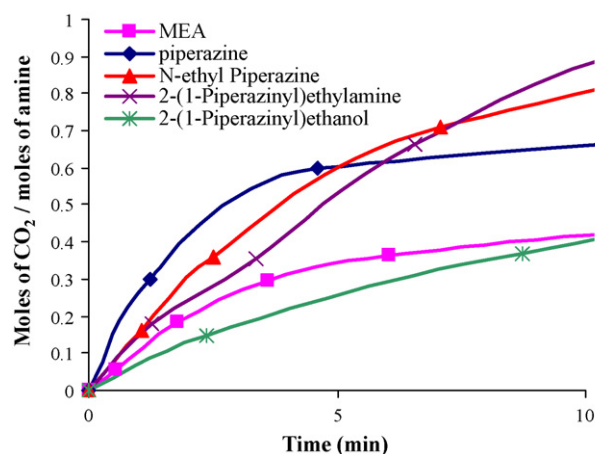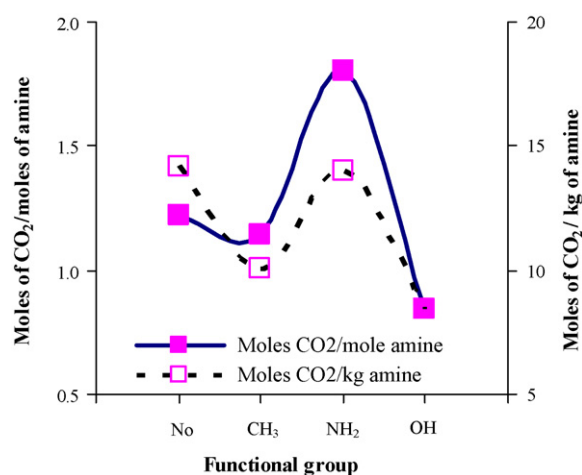**Fig. 21 – Influence of number of alkyl group on total loading for CO_2 absorption.**

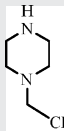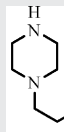**Table 7 – Total capacity of aqueous cyclic diamine-based absorbents: A (moles CO₂/moles amine); B (moles CO₂/kg amine)**

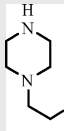| Aqueous absorbent	CO₂ loading	
	A	B
Piperazine	1.22	14.20
1-Methyl piperazine	1.12	11.23
Trans piperazine, 2,5-dimethyl	1.28	11.19

increasing the absorption rate. Furthermore, the substituted methyl group has a highly electronegative function, which can favor the accessibility of the lone-pair electrons of the amine group for CO_2.

From Fig. 21 and Table 7, it is clear that the absorption capacity with a one methyl group substituted cyclic diamine (2-methyl piperazine) is slightly lower when compared with a 2 methyl group substituted cyclic diamine (*trans*-piperazine 2,5-dimethyl: 1.12 and 1.28 moles CO_2/moles amine, respectively). Substitution of 2 methyl group on saturated cyclic amines reduces the initial absorption rate, but the absorption capacity is increased.

The effect of different functional groups in aromatic diamines was also investigated. The concentration of *N*-ethylpiperazine, 2-(1-piperazinyl) ethylamine and 2-(1-piperazinyl) ethanolamine was kept to be at 1 mol/l. Figs. 22–24 and Table 8 shows the effect of a substitution with an amine, alkyl and hydroxyl group on the saturated diamine. Figs. 22 and 23 show that substitution with an amine and

Fig. 22 – Influence of a side chain on saturated cyclic diamine for the absorption of CO_2 in aqueous absorbents.

Fig. 23 – Influence of number of alkyl group for the absorption of CO_2 in aqueous absorbents.

Fig. 24 – Influence of number of alkyl group on total loading for CO_2 absorption.

Table 8 – Total capacity of aqueous amine-based absorbent: A (moles CO₂/moles amine); B (moles CO₂/kg amine)
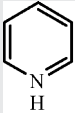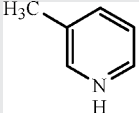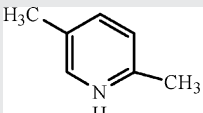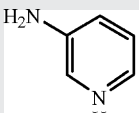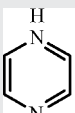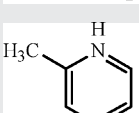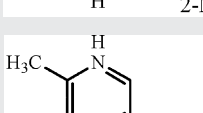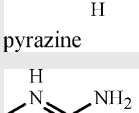
Aqueous absorbent	CO₂ loading	
	A	B
N-ethylpiperazine	1.15	10.03
2-(1-Piperazinyl) ethylamine	1.81	13.97
2-(1-Piperazinyl) ethanol	0.84	8.41

alkyl group in saturated diamines slightly increased the initial absorption rate after 5 min of the CO_2 absorption time. Substitution with an amine or alkyl group on the saturated diamine increased the initial absorption rate, whereas substitution with a hydroxyl group caused a decrease in the initial absorption rate.

The absorption capacities of the saturated diamines substituted with an amine, alkyl or hydroxyl group were 1.81, 1.15 and 0.84 moles CO_2/moles amine, respectively. From these results it is clear that an alkyl or amine group substitution in saturated diamine is most suitable for an improved CO_2 absorption capacity as well as absorption rate.

Unsaturated cyclic amines were also investigated (see Table 9). All compounds showed a poor absorption rate and capacity. However, upon substitution with a methyl group at the 2nd or two alkyl groups at the 2nd and 5th position in the saturated amines, an increase in the absorption capacity was found. Unsaturated amines substituted with an amine group

Table 9 – Total capacity of various aqueous unsaturated cyclic amine-based absorbent (moles CO_2/moles amine)

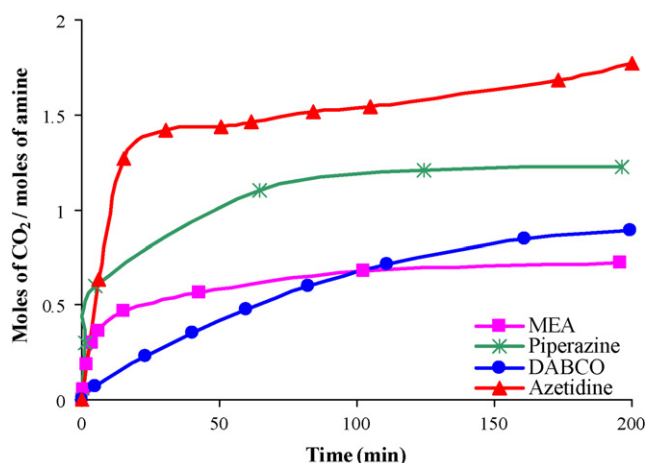| Aqueous absorbent	CO_2 loading
Pyridine	0.05
2-Pyridylamine	0.28
2-,5-Lutidine	0.29
2-Methyl pyridine	0.06
Pyrazine	0.04
2-Methyl pyrazine	0.10
2.5-Dimethyl pyrazine	0.11
Aminopyrazine	0.12

Fig. 25 – Influence of the different structures for the absorption of CO_2 in aqueous absorbents.

as the side chain (i.e. aminopyrazine) showed an increase in the absorption capacity.

Finally, the effect of different ring shapes was investigated. The concentration of azetidine and DABCO was 0.1 mol/l and 2.5 mol/l respectively. Figs. 25–27 and Table 10 shows that the small ring in azetidine result in a very high absorption capacity of upto 1.77 moles CO_2/moles amine. Azetidine absorption
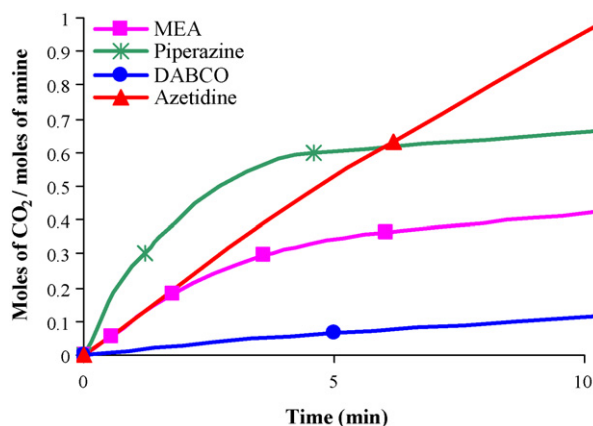

Fig. 26 – Influence of different ring structure for the absorption of CO_2 in aqueous absorbents.
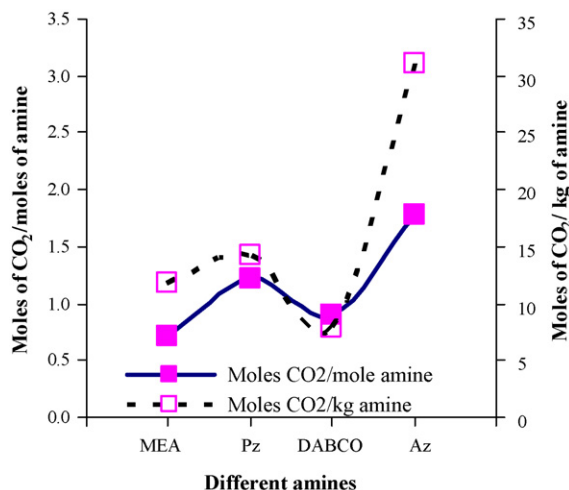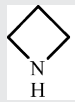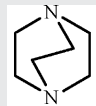

Fig. 27 – Influence of different structure on total loading for CO_2 absorption (Pz, piperazine; Az, azetidine; DABCO, 1,4-diazabicyclo[2,2,2]octane).

Table 10 – Total capacity of aqueous amine-based absorbents: A (moles CO_2/moles amine); B (moles CO_2/kg amine)

Aqueous absorbent	CO_2 loading	
	A	B
Azetidine	1.77	31.03
DABCO Or 1,4-Diazabicyclo [2.2.2]octane	0.89	7.95

capacity was higher than mono saturated amine (piperidine) with upto 1.26 moles CO_2/moles amine and for saturated diamine (piperazine) 1.22 moles CO_2/moles amine. This might be caused by the fact that the azetidine molecule is very small and can adopt a spatial arrangement in the solution that favours the accessibility of the loan-pair electrons of the nitrogen atom for CO_2. When comparing the absorption capacity in unit of moles CO_2/kg amine azetidine showed very high CO_2 absorption rates of upto 31.03 moles CO_2/kg amine. DABCO showed lower absorption capacities of upto 0.89 moles CO_2/moles amine when compared with a saturated diamine (Piperazine) 1.22 moles CO_2/moles amine. The low absorption capacity in DABCO might be caused by the presence of a bond between the two amine groups present in the saturated diamine ring. This might result in a slower hydrolysis reaction and hence in a lower absorption capacity.

Figs. 25 and 26 shows that the small ring absorbent azetidine has a faster initial absorption rate compared with DABCO and MEA. Still the azetidine initial absorption rate was slower than for piperazine.

The effect of other functional groups on amine-based absorbents was also studied, e.g. ketone, aldehyde, ester, amide, etc. All of these showed very poor absorption rates and capacities.

4.   Conclusions

The present study revealed the structural effects of various amine-based absorbents on the initial CO_2 absorption rate and capacities. Alkyl and amine groups were found to be most suitable substituted functional groups to enhance the absorption rate and capacity of amine-based absorbents. Substitution of hydroxyl groups decreased the initial absorption rate and increased the capacity. In cyclic saturated and unsaturated amine basicity was increased by substituting with alkyl groups at the 2nd and 5th position in the ring. This increased the initial absorption rate and capacity in these amine-based absorbents. Substitution of the alkyl and amine group by a side chain in saturated cyclic amines increased both the capacity and initial absorption rate. Unsaturated amines showed poor absorption rates and capacities for CO_2 absorption. A substitution with an alkyl group at the 2nd and 5th position in a saturated cyclic amine resulted in enhanced absorption capacity. This study will be advantageous in the development of an improved amine-based CO_2 absorbent, leading to a better approach for the development of new technologies in the CO_2 capture area.

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