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# Analysis of $CO_2$ solubility and absorption heat into aqueous 1-Diethylamino-2-propanol

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## Abstract

In this work, the $CO_2$ equilibrium solubility in 2M 1-diethylamino-2-propanol (1DEA2P) solution were determined as function of temperature (in the range of 298-333K), and $CO_2$ partial pressure (in the range of 8-101kPa). The modified Li-shen $K_2$ correlation model was also developed and used to predicate the $CO_2$ equilibrium solubility in 1DEA2P solution. with an excellent ADD of 3.4%. The heat of $CO_2$ absorption in 1DEA2P solution estimated using Gibbs-Helmholtz equation was found to be -45.7 kJ/mol. In addition, the ion (1DEA2P, 1DEA2PH$^+$, HCO$_3^-$, CO$_3^{2-}$) speciation plots of the 1DEA2P-$CO_2$-$H_2O$ system were developed in order to further understand the reaction process of 1DEA2P with $CO_2$.

*Keywords:Equilibrium $CO_2$ solubility, Liu-Helei model, Ion speciation plots, 1DEA2P, $CO_2$ absorption.*

## 1. Introduction

As the global warming becomes one of the issues of greatest concern, $CO_2$ was considered as a major greenhouse gas which make a most contribution to the global warming.[1]

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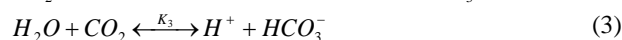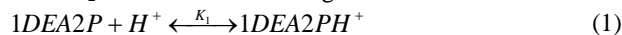*E-mail address:*paitoon@uregina.ca

Therefore, the research on decrease of the emission of $CO_2$ is becoming more and more urgent.$CO_2$ capture is considered as one of most effective method to reduce the $CO_2$ emission. The absorption using the aqueous solutions of alkanolamines is the most widely used technology for capturing $CO_2$ from the gas streams in industrial processes due to its characteristics of mature technique, good economic effectiveness, and ability to deal with large scales of streams.[2, 3] However, one of the most sticking point for this technique is using a high-performance absorbent, which should meet the basic requirements, such as large absorption capacity, fast reaction kinetics, good solvent stability, and energy efficiency for the regeneration[4, 5]. As the previous study,[6] DEAB exhibited a high $CO_2$ absorption capacity, a fast reaction kinetics, and a fast mass transfer. A new tertiary amine, 1-diethylamino-2-propanol (1DEA2P), has the extremely similar structure as DEAB. Thus, 1DEA2P could show a good performance on $CO_2$ capture as 1DEA2P.

However, there are very few articles providing detailed information and no further research about the $CO_2$ capture performance of 1DEA2P, such as solubility, reacting kinetics, heats of reaction, mass transfer. Before being used for commercial application, those characteristics should be comprehensively figured out. Besides, the reliable vapor-liquid equilibrium (VLE) data is another essential considerable parameter, since it can provide quantitative information on the $CO_2$ absorption, kinetics behavior and mass transfer.

In this present work, the performances of $CO_2$ absorption into aqueous 1DEA2Psolution were comprehensively investigated in the terms of the $CO_2$ equilibrium solubility, and the absorption heat. the $CO_2$ equilibrium solubility in 2M 1-diethylamino-2-propanol (1DEA2P) solution were determined as function of temperature (in the range of 298-333K), and $CO_2$ partial pressure (in the range of 8-101kPa). The new modified $K_2$ correlation model was modified based on the Li-shen model by adding another factor the total pressure, which was developed by the Liu et al[7]. In this work, this modified model was also developed and used to predicate the $CO_2$ equilibrium solubility in 1DEA2P solution. The heat of $CO_2$ absorption in 1DEA2P solution estimated using Gibbs-Helmholtz equation. In addition, the ion (1DEA2P, $1DEA2PH^+$, $HCO_3^-$, $CO_3^{2-}$) speciation plots of the 1DEA2P-$CO_2$-$H_2O$ system were developed in this work.

## 2. Theory

As the base-catalyzed hydration mechanism shows,[8] the tertiary amine does not react directly with $CO_2$but it acts as a base that catalyzes the hydration of $CO_2$. Since 1DEA2P is a tertiary amine, the reaction between 1DEA2P and $CO_2$ can be described using this mechanism as shown in the following equations:

$$1DEA2P + H^+ \xleftrightarrow{\phantom{x}K_1\phantom{x}} 1DEA2PH^+ \qquad (1)$$

$$CO_2 + 1DEA2P \xleftrightarrow{\phantom{x}K_2,k_2,k_{-2}\phantom{x}} 1DEA2PH^+ + HCO_3^- \qquad (2)$$

$$H_2O + CO_2 \xleftrightarrow{\phantom{x}K_3\phantom{x}} H^+ + HCO_3^- \qquad (3)$$

$$CO_2 + OH^- \xleftrightarrow{\phantom{x}K_4\phantom{x}} HCO_3^- \qquad (4)$$

$$HCO_3^- \xleftrightarrow{\phantom{x}K_5\phantom{x}} H^+ + CO_3^{2-} \qquad (5)$$

$$H_2O \xleftrightarrow{\phantom{x}K_6\phantom{x}} H^+ + OH^- \qquad (6)$$

where $K_i$ represent the chemical equilibrium constants of the reaction*i*.

In this system of 1DEA2P-$H_2O$-$CO_2$, there are several equilibrium constants for chemical reactions, which can be

presented as follows:

$$K_1 = \frac{[1DEA2PH^+]}{[1DEA2P][H^+]} \qquad (7)$$

$$K_2 = \frac{[1DEA2PH^+][HCO_3^-]}{[CO_{2(aq)}][1DEA2P]} \qquad (8)$$

$$K_3 = \frac{[H^+][HCO_3^-]}{[CO_{2(aq)}]} \qquad (9)$$

$$K_4 = \frac{[HCO_3^-]}{[CO_{2(aq)}][OH^-]} \qquad (10)$$

$$K_5 = \frac{[H^+][CO_3^{2-}]}{[CO_{2(aq)}][HCO_3^-]} \tag{11}$$

$$K_6 = [H^+][OH^-] \tag{12}$$

From the equations 7-12, there is a correlation between these equilibrium constants and only four constants ($K_1$, $K_3$, $K_5$, and $K_6$) are independent. $K_1$ can be extracted from the work of Liu et al.,[9] $K_3$, $K_5$, and $K_6$ can be found from the literature. [10-12]

Several balance equations exist in the system of 1DEA2P-$H_2O$-$CO_2$, which can be shown as follows:

The mass balance of 1DEA2P:

$$[1DEA2P]_0 = [1DEA2PH^+] + [1DEA2P] \tag{13}$$

The mass balance of carbon:

$$\alpha[1DEA2P]_0 = [CO_{2(aq)}] + [HCO_3^-] + [CO_3^{2-}] \tag{14}$$

The charge balance:

$$[1DEA2PH^+] + [H^+] = [OH^-] + [HCO_3^-] + 2[CO_3^{2-}] \tag{15}$$

where $[1DEA2P]_0$ is the initial 1DEA2P concentration(mol/L)and *a* represents the $CO_2$ loading (mol $CO_2$/mol amine).

### 2.1. CO₂ absorption heat in aqueous 1DEA2P solutions

In the evaluation of new alternative solvents for the capture of $CO_2$, the heat of $CO_2$ absorption is one of the most important factors to consider due to its close relationship to regeneration energy. The heat of $CO_2$ absorption can be obtained by the experimental method with a calorimeter. In addition, the heat of $CO_2$ absorption also can be estimated by application of the Gibbs-Helmholtz equation[13] as shown in eq16:

$$\frac{d\left(\ln P_{CO_2}\right)}{d\left(\frac{1}{T}\right)} = \frac{\Delta H_a}{R} \tag{16}$$

where $\Delta H_a$ is the heat of $CO_2$ absorption (J/mol), and R represents the universal gas constant (J/mol K).

### 2.2. Calculation of the concentration of ions in the 1DEA2P-CO₂-H₂O system

The ion speciation plots are of prime importance for comprehensively understanding the reaction process of aqueous amine solutions with $CO_2$. In order to develop ion speciation plots of the1DEA2P-$CO_2$-$H_2O$ system, all the ion concentrations (1DEA2P, 1DEA2PH$^+$, HCO$_3^-$, CO$_3^{2-}$) should be presented in detail. These ion concentrations can be calculated with the mass balance equations (eq.13 and eq.14), the equilibrium constant equations (eq.7, eq.11 and eq.12), and charge balance equations (eq. 14) and the concentration of H$^+$. The H$^+$ concentration can be calculated by equation 17:

$$pH = -\log(H^+) \tag{17}$$

## 3. Experimental section

### 3.1. Chemical

1-diethylamino-2-propanol (1DEA2P) with a purity of 97% was purchased from Alfa-Chemistry, American. MDEA with a purity of ≥99% was obtained from Tianjin Hengxing Chemical Preparation Co., Ltd, China. The desired concentrations of amine solutions were obtained by dilution of deionized water. $N_2$ and $CO_2$cylinders with purities of 99.9% were provided by Changsha Jingxiang Gas Co., Ltd., China.

### 3.2. CO₂ equilibrium solubility

The apparatus used to measure the $CO_2$ solubility of 1DEA2P in this work is similar to our previous work. Briefly.

this equipment is mainly made up of a saturation cell, an absorption reactor, a mass flow meter, and a water bath with a temperature controller. For each experiment, the saturated cell and the absorption reactor were immersed in a water bath equipped with a temperature controller. Then, a gaseous stream with desired $CO_2$ concentration was passed through a water saturation cell and then bubbled into the liquid amine sample. This condition was kept for 8-10 hours in order to obtain the equilibrium $CO_2$ loading condition. Then, this liquid sample is taken to measure $CO_2$ solubility. The amine concentrations and the $CO_2$ solubility were determined by titration with a 1M HCl solution. All operations of measurement for equilibrium $CO_2$ solubility were conducted at the atmosphere.

## 4. Results and discussion

### 4.2. $CO_2$ equilibrium solubility of 1DEA2P solution

The equilibrium solubility of $CO_2$ represents the maximum $CO_2$ amount that can be absorbed in amine solutions, and is a great parameter to evaluate a new solvent. Thus, the study on the equilibrium solubility of $CO_2$ in 1DEA2P solutions is of significance. In this work, the equilibrium solubility of $CO_2$ in 2 M 1DEA2P aqueous solutions was measured over a temperature range of 298-333 K, and a $CO_2$ partial pressure range of 8.0-101.3 kPa. All the experimental results are plotted in Figure1,and show that 1DEA2P has a very high $CO_2$ absorption capacity. Figure 1 clearly shows that the equilibrium solubility of $CO_2$ increased with the increase in $CO_2$ partial pressure. Besides that, the equilibrium solubility of $CO_2$ decreased with increasing temperature, the same trend as reported by Kundu et al.[14] This is mainly because the higher temperature leads to faster molecular motion, which makes $CO_2$ molecules in the solution less likely to remain combined with the 1DEA2P molecules. When the $CO_2$ partial pressure was raised, this increased the mass transfer driving force of gas phase due to the increase of the concentration gradient, which promoted the increase of $CO_2$ solubility. Meanwhile, the increase of $CO_2$ partial pressure leads the physical dissolution equilibrium to shift toward the right side (reaction 2). As a result, the equilibrium solubility of $CO_2$ increased with increasing$CO_2$ partial pressure.
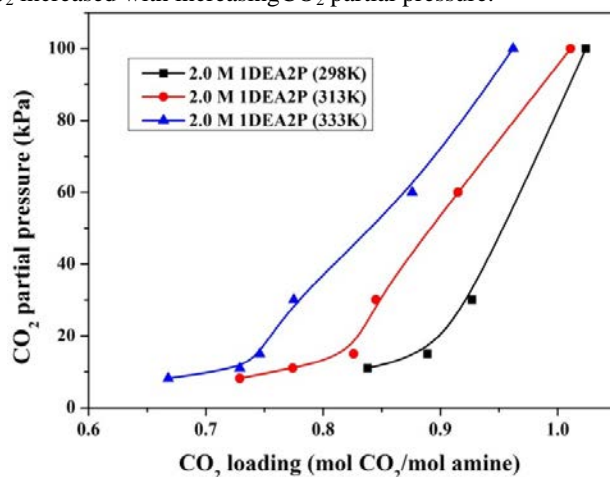


**Figure 1.**$CO_2$equilibrium solubility of in 2M aqueous 1DEA2P solution at 298, 313, and 333 K.

### 4.2. Ion speciation plots of 1DEA2P-H$_2$O-CO$_2$ system

The concentration of ions in the systems of amine-$CO_2$-$H_2O$ is significant in the comprehensive understanding of the reaction process of amine with $CO_2$. In this work, the concentrations of the cations and anions ([1DEA2P], [1DEA2PH$^+$], [$HCO_3^-$], [$CO_3^{2-}$]) in the system of 1DEA2P-$CO_2$-$H_2O$ were calculated by combining the equilibrium constants ($K_1$, $K_3$, $K_5$ and $K_6$), eqs 13-15, the initial concentration of 1DEA2P ([1DEA2P]$_0$; mol/L), pH values, and the$CO_2$ loading of 1DEA2P ($a$, mol $CO_2$/mol amine).

Based on the results of ion concentrations, the ion speciation plots of the 1DEA2P-$CO_2$-$H_2O$ system were developed at the temperatures of 298K, 1DEA2P concentration of 1M, and at $CO_2$ loading range of 0-0.8 mol $CO_2$/

mol amine. All the results are plotted and presented in Figure 2.From Figure 2, it is clearly seen that concentrations of free 1DEA2P decreased with the increasing $CO_2$ loading, which is mainly caused by the reaction of1DEA2P solution with $CO_2$ and the appearance of the 1DEA2P protonation. As a result, the concentration of 1DEA2PH$^+$(protonated 1DEA2P) increased gradually with the increase in $CO_2$ loading. As one of the principal products, $HCO_3^-$ increased as the $CO_2$ loading increased. However, the $CO_3^{2-}$ (another product) concentration was not straightforward, as it increased with the increased $CO_2$ loading at low $CO_2$ loading but then after reaching a maximum, it decreased with the increase in $CO_2$ loading. The reason was that at very low loadings, the strong basicity of the solution due to the excess of 1DEA2P accepted the protons and generated $CO_3^{2-}$, so the concentration of $CO_3^{2-}$ increased at the lean $CO_2$ loading. As a result, $CO_3^{2-}$ was observed to be a major component rather than $HCO_3^-$ at the lower $CO_2$ loading. However, as the $CO_2$ loading increased, the solution basicity became weaker because of the decrease of free 1DEA2P. This led $CO_3^{2-}$ to accept protons and convert to $HCO_3^-$ through equation 5, which results in a phenomenon of a decrease in $CO_3^{2-}$concentration and $HCO_3^-$ becoming the major component rather than $CO_3^{2-}$.

In addition, the NMR technique is another technique that is always employed to develop the ion speciation plots. In comparison with NMR technique,[15] the pH method used in this work has several advantages. This method is simple and convenient because it can entirely determine the exact concentrations of $HCO_3^-$, $CO_3^{2-}$, free 1DEA2P and 1DEA2PH$^+$ in the 1DEA2P-$CO_2$-$H_2O$ system independently by using the pH values. However, the disadvantage of this method is that it can only applied at lower temperatures.
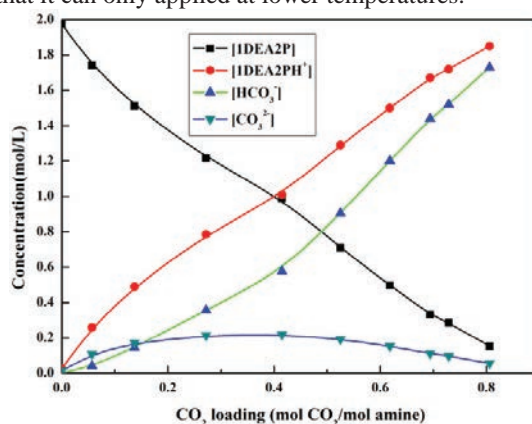


**Figure 2.**Ion speciation plots in 1DEA2P-$H_2O$-$CO_2$ system at 298K.

### 4.3. Modified Li-shen model

As well known, the chemical equilibrium constants are closely related to the chemical reaction[6]. Thus, the parameters affecting the chemical reaction played the vital roles in the chemical equilibrium constants. It is generally accepted that the total pressure, temperature, $CO_2$ loading, free amine concentration and physical $CO_2$ solubility affect the chemical reaction of $CO_2$ with amine. In order to better predicate the $CO_2$ equilibrium solubility in 1DMA2P solution, it is reasonable to add all of the total pressure, temperature, $CO_2$ loading, free amine concentration and physical $CO_2$solubilityin the model for correlation $K_2$. Thus, the new model, modified Li-shen model, was developed by adding all of the total pressure, temperature, $CO_2$ loading, free amine concentration and physical $CO_2$ solubility, which was shown as following equation:

$$K_i = \exp(E_1 + E_2 T + E_3 [CO_{2aq}] + E_4 \ln[Amine] + E_5 \alpha + E_6 P_{total}) \tag{21}$$

where $P_{total}$ is total pressure of the reaction system, $[CO_{2aq}]$ is the physical solubility of $CO_2$ in aqueous 1DEA2P solution, which could be expressed by the equation of ($[CO_{2aq}]=P_{CO2}/He_{CO2}$).

This new model was also used to correlate the experimental $CO_2$ equilibrium solubility of 1DMA2P solution in order to achieve the parameters ($E_1$, $E_2$, $E_3$, $E_4$, $E_5$ and $E_6$) in the proposed new model. All the determined values of parameters are shown in Table 1. As in the previous models, the correlation for $K_2$ in proposed new model was applied to represent the $CO_2$ equilibrium solubility. In addition, all the predicted and experimental results of $CO_2$

equilibrium solubility in 1DEA2P solution were also provided in this work. It can be founded that the predicated results have a good agreement with the experimental values with an acceptable AAD of 3.4%.

**Table 1.** Values of Parameters for modified Li-shen model

| Parameters for $K_2$ | Values |
|---|---|
| $E_1$ | -48.999 |
| $E_2$ | 0.0392 |
| $E_3$ | 1.000 |
| $E_4$ | -0.000624 |
| $E_5$ | 90.999 |
| $E_6$ | 0.9999 |

*4.3. Heat of $CO_2$ absorption in aqueous 1DEA2P solution*

The heat of $CO_2$ absorption is another significant factor to consider due to its close relationship to the energy requirement for regeneration of the amine in the $CO_2$ removal process. In the work of Carson et al.,[16] the experimental heats of $CO_2$ absorption of MEA, DEA, and MDEA were obtained using the experimental method (calorimeter) and the $CO_2$ absorption heat was estimated using the Gibbs-Helmholtz equation(eq. 18). The experimental and estimated results for MEA,[17] DEA,[18] and MDEA [19]are presented in Table 2. By comparison of the results extracted from the two methods, it is found that the estimated results on the basis of the Gibbs-Helmholtz equation have an excellent agreement with the experimental results. Therefore, using the Gibbs-Helmholtz equation to estimate $CO_2$ absorption heat is relatively reliable.

In this work, the heat ($\Delta H_a$) of $CO_2$ absorption in aqueous 1DEA2P was estimated to be -43.6 kJ/mol by using the Gibbs-Helmholtz equation. In comparison with conventional amines (MEA, MDEA, and DEA) and the alternative amines (DEAB, 1DMA2P), it was found that the heat of $CO_2$ absorption for 1DEA2P is distinctly lower than that in MEA, DEA, and MDEA, and higher than that in 1DMA2P and DEAB. This is mainly because the bonding strength for $CO_2$ with 1DEA2P is less than that for the secondary amine (DEA) and the primary amine (MEA),which indicates that the reaction heat of 1DEA2P is less than the other amines.[13]

**Table 2.** $CO_2$ absorption Heat in Aqueous Solution of MEA, DEA, MDEA, DEAB, 1DMA2P and 1DEA2P.

| Amine | $\Delta H_a$ (kJ/mol) | |
|---|---|---|
| | Estimated | Experimental |
| MEA | -84.3 | -82 |
| DEA | -66.9 | -69 |
| MDEA | -54.6 | -49 |
| 1DMA2P | -30.5 | N/A |
| DEAB | -41.4 | N/A |
| 1DEA2P | -43.6 | N/A |

## 5. Conclusion

In this work, the $CO_2$ equilibrium solubility in 2M 1-diethylamino-2-propanol (1DEA2P) solution were determined as function of temperature (in the range of 298-333K), and $CO_2$ partial pressure (in the range of 8-101kPa). The new modified $K_2$ correlation model, was also developed and used to predicate the $CO_2$ equilibrium solubility in 1DEA2P solution. with an excellent ADD of 3.4%. In addition, the heat of $CO_2$ absorption in 1DEA2P solution was estimated to be -45.7 kJ/mol by using Gibbs-Helmholtz equation. In addition, the ion (1DEA2P, 1DEA2PH$^+$, HCO$_3^-$, CO$_3^{2-}$) speciation plots of the 1DEA2P-$CO_2$-$H_2O$ system were developed in order to further understand the reaction process of 1DEA2P with $CO_2$.

## Acknowledgements

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