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Original Research Article

In Vitro Study of Solubility of Carbon Dioxide in Diethyl Ethanolamine in the Presence of Calcium Carbonate Nanoparticles

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ABSTRACT

In this study carbon dioxide solubility in diethyl ethanolamine (DEEA) solvent with and without the presence of calcium carbonate nanoparticles at concentrations of 10, 15 and 20 wt% solvent in the pressure range of 5, 10 and 15 bar and titanium oxide, respectively. At concentrations of 0.05 and 0.1 wt% were measured at ambient temperature. The results show that at constant pressure (10 bar) and without the presence of nanoparticles, the solubility for the concentration of 10 to 15 wt% of the solvent increases from 26.03 v/v* to 42.28 v/v*. Increasing the pressure also increases the solubility. For a constant concentration (15 wt% of the solvent), the solubility increases from 24.38 v/v* to 34.66 v/v* by increasing the pressure from 10 to 15 times. So that for the constant concentration of solvent (15%) and constant pressure (15 bar) the solubility of carbon dioxide for the nanoparticles increases from 0 to 0.1

Keywords: Solubility, Calcium Carbonate Nanoparticle, Carbon Dioxide, Diethyl Ethanolamine

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Introduction

Fossil fuels are a major source of carbon dioxide emissions into the atmosphere, which are sources of air pollutants [1]. Various countries have taken various measures to reduce the amount of CO_2 that accumulates in greenhouse gases and warms the air, elevating seas, droughts and acid rain [2]. Carbon dioxide removal is important not only from an environmental perspective but also in industry, including in the process of ammonia production, hydrogen production and natural gas sweetening [3]. Physical adsorption, chemical adsorption, membrane separation, molecular sieving, and cryogenic distillation methods are among the industrial methods used to remove carbon dioxide gas [4]. Chemical adsorption processes using amine solvents and physical adsorption are widely used in industries to absorb acid gases such as CO_2 and H_2S. In such processes, physical absorption is preferable when the partial pressure of the acidic gases in the gas stream is relatively high. Chemical adsorption using alkanes is used to increase gas absorption rate, capacity and selectivity [5-7]. MEA and DEA have been widely used during the past decade, however, these amines require high regeneration energy, leading to high costs for the CO_2 capture process. Methyl di-ethanolamine is a third type of amine which has advantages such as lower vapor pressure, lower reaction heat and higher thermal stability than other amines. Also, methyl di-ethanolamine does not degrade easily, so it cannot cause corrosion [5-7].

On the other hand, much research has been done in the field of nanotechnology, especially in the field of nanofluids. Nanotechnology for adsorption systems can be used to enhance heat transfer and mass transfer performance [8]. The use of nanoparticles as fluid additives to improve mass transfer has attracted the attention of many researchers for its application in the adsorption process. So much of the research that has been done so far has shown that increasing the nanoparticles to the solvent can increase the mass transfer intensity. In 2018, Morteza Afkhami *et al.,* Optimized a model for CO_2 absorption capacity by new amine solvents: 1-DEMA, DEEA, $1DEA_2P$, $DEMA_2P$, they developed a model for the evaluation of CO_2 adsorption by tertiary amines called 1-diethylamino-2-propanol (1-DMA_2P,), 1-diethylamino-2-propanol (1 $DEA2P)_2$-diethylaminoethanol (DEEA). And 4-diethylamino-2-butanol (DEAB).

They used the Kent-Eisenberg model, the modified K-E (M-E-K) model, and the De-nshmukh-Mather (DM) model to predict CO_2 absorption by amine solvents. They found that the DM model was superior to the MEK and KE models with an absolute relative average deviation (AARD) of

2.36% compared to the thermodynamic models for all the investigated amines (DEEA, 1DMA2P, DEAB, 1DEA2P) [9]. S. ADAK *et al.*, 2017, Solubility of carbon dioxide in aqueous solution of diethyl amino ethanol and Piperazine (DEAE + PZ) in the low pressure range between 65-0.1 KP and temperature range 323.15-303.15 Kelvin examined. The results show that PZ + DEAE combines better and more CO2 than MDEA + PZ [10].

In 2016, Dong Fu *et al.*, measured the CO_2 absorption capacity in Piperazine aqueous solution (PZ) expanded to 2-diethylaminoethanol (DEAE). The viscosity of DEAE-PZ aqueous solution was measured in both loaded and unloaded CO_2 states. As the amount of CO_2 absorption increases, the viscosity increases uniformly and as the temperature increases, the viscosity decreases exponentially [11]. In 2016, Hossein Shahraki *et al.*, Investigated the solubility of CO_2 in Piperazine-activated methyl di-ethanolamine (MDEA) adsorption and desorption processes with 12, 25, 50 and 100 ppm nanoparticles. The study showed that adding 25 ppm of activated nanoparticles to MDEA increased the CO_2 uptake by 37.5% compared to the nanoparticle Free State. In a process of CO_2 capture based on nanoparticles, approximately 37.5% of the solvent flow is reduced, thus the process in which the nanoparticles are adsorbed is much better economically and efficiently [12].

Theory and Computation

In order to perform the solubility calculations, a state equation is needed which uses the Peng-Robinson equation in this study. The Peng-Robinson equation of state was proposed by Peng-Robinson in 1976, in which the parameters of the state equation are obtained by the critical properties and the decay coefficient [13].

$$P=\frac{RT}{v-b}-\frac{a}{v(v+b)+b(v-b)} \qquad (1)$$

In order to do the calculations, we have to rewrite the equation of state in terms of the Z compressibility coefficient, which is obtained by using the Peng-Robinson equation of state (2) in Z.

$$Z^3-(1-B)Z^2+(A-2B-3B)Z-(AB-B^2-B^3)=0 \qquad (2)$$

$$A = \frac{a\alpha P}{R^2 T^2} \quad (3)$$

$$B = \frac{BP}{RT} \quad (4)$$

$$a=0.457235\frac{(RT_C)^2}{P_C} \quad (5)$$

$$b=0.077796\frac{RT_C}{P_C} \quad (6)$$

$$\alpha = [1+ (0.37464+1.54226\omega-0.26992\omega^2) (1+T_r^{0.5})]^2 \quad (7)$$

$$T_r=\frac{T}{T_C} \quad (8)$$

In the above equations, the molar volume, TC and PC are the temperature and pressure at the critical point, respectively, the global constant R of the gases and the centroid coefficient ω. By solving equation (2) in the vapor-liquid calculations, the resulting Z is used for the vapor phase and the lowest value for the liquid phase. Using Z obtained at the initial and equilibrium temperature and pressure, the number of primary and equilibrium moles is obtained from equations (9) and (10) [14]:

$$n_0 = \frac{P_0 V_0}{Z_0 R T_0} \quad (9)$$

$$n_e = \frac{P_e V_e}{Z_e R T_e} \quad (10)$$

$$\Delta n = n_0 - n_e \quad (11)$$

The equation (11) defines solubility in mole of carbon dioxide relative to kg of solvent. To calculate the mole fraction of dissolved carbon dioxide in the solvent using the volumetric method, use in which the standard volume is calculated by the following equation [12]:

$$V_{STP} = \frac{nRT}{p} \quad (12)$$

In Equation (14), the volume of carbon dioxide gas is calculated under standard conditions (means atmospheric pressure and temperature of 25 ° C).

Experiments

Device: For the experiments, a jacket-type (fixed-volume) reactor made of stainless steel 316 (SS-316) with an internal volume of 296 cm^3, which withstands operating pressure of 200 bar, was used. The inner chamber of this reactor is equipped with four valves with a pressure of 6000 psi, two of which are ball valves used for solution injection as well as discharge of water and gas mixture after the test, and the other two are needle valves, one for gas injection and the other for gas chromatography and gas sampling. There is also a gas loading chamber with a volume of 1820 cm^3 with two ball valves, one for injection and the other for discharge into the reactor. To measure the temperature inside the reactor, a Pt-100 platinum temperature sensor with an accuracy of K 0.1 K was used. The tank pressure was measured with a BD sensor with an accuracy of about 0.01 MPa. A stirring mixer was used to create the proper mixing in the absorption tubes and a pump was used to create the vacuum inside the tubes. A schematic of the hydrate forming device used in this study is shown in Fig. (1).

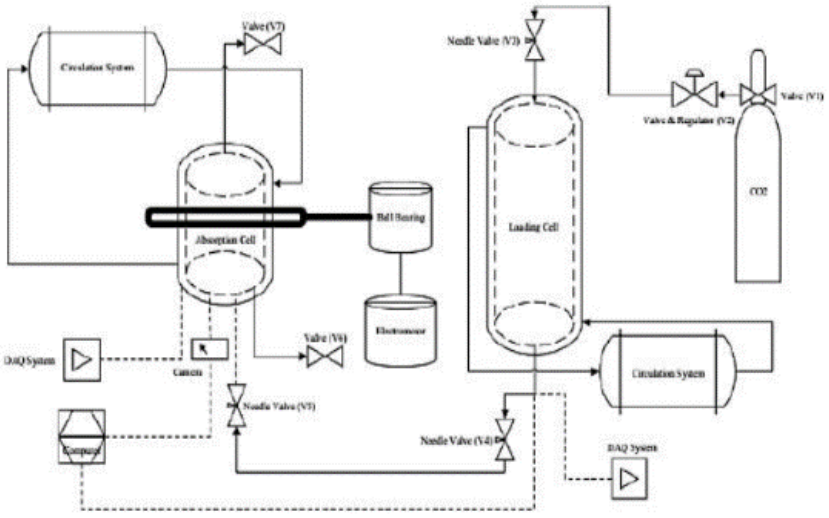

Figure 1. Schematic of the device used in this work

Materials: Materials used in this work include carbon dioxide gas with a purity of 99.99% prepared by Arvand Industrial Gas Company, calcium carbonate nanoparticle as a solvent suspended particle and effective absorption factor in some formulation experiments $CaCO_3$ chemicals are from Nano Pasargad Novin, 2-DEEA (99.99% purity) from Fouca Swiss Company with $C_6H_{15}NO$ chemical formula and DM (Demineralized Water) for solution preparation.

Results and Discussion

In this study carbon dioxide solubility in DEEA solution in the presence and absence of calcium carbonate nanoparticles with different concentrations and pressures was measured and the experimental results are presented in this section.

Evaluation of solubility of carbon dioxide using Peng-Robinson state equation: In order to investigate the real behavior of carbon dioxide solubility in diethyl ethanolamine, its solubility has been calculated using Peng-Robinson equation. The results of these calculations are presented in Table (1).

Table (1). Carbon dioxide solubility results using Peng-Robinson state equation

RUN	Solvent(AMIN)	Nano particle	P_0	V(STP)	X
1	20	0	9	4227.99	42.28
2	15	0	13.5	3270.66	32.71
3	15	0	4.5	3253.49	32.53
4	10	0	9	2603.68	26.04
5	20	0.05	13.5	4049.25	40.49
6	20	0.05	4.5	3779.87	37.80
7	15	0.05	9	3360.06	33.60
8	10	0.05	13.5	2476.68	24.77
9	10	0.05	4.5	1718.72	17.19
10	20	0.1	9	3941.32	39.41
11	15	0.1	13.5	3466.13	34.66
12	15	0.1	4.5	2437.91	24.38
13	10	0.1	9	2321.82	23.22

As shown in Table (1), the solubility of carbon dioxide in water without the presence of nanoparticles increases with increasing solvent concentration of amine. And if the nanoparticles are added to the solution, the solubility will continue to increase. Further, through the graphs, further investigation and interpretation of solubility changes in the presence of nanoparticles and

solvents are discussed.

Influence of different parameters on solubility: In diagrams (1) to (6), the effect of each of the parameters (pressure, Nano-particle and solvent) on the solubility of carbon dioxide, as shown in Table (1), can be seen simultaneously.

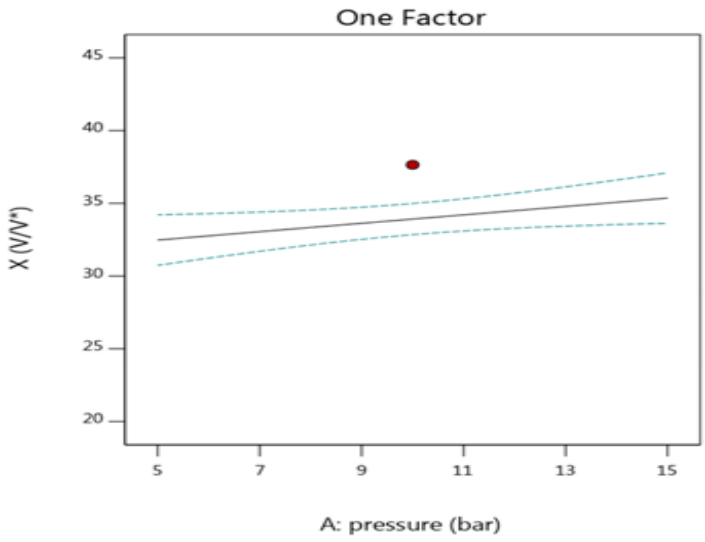

Diagram 1. The effect of pressure on solubility

Diagram (1) shows the impact of pressure on carbon dioxide solubility. The effect of pressure on the solubility of CO_2 for nanoparticles with a concentration of 0.05 wt% and a solvent with 15 wt% shows. Which has less effect on CO_2 solubility than solvent.

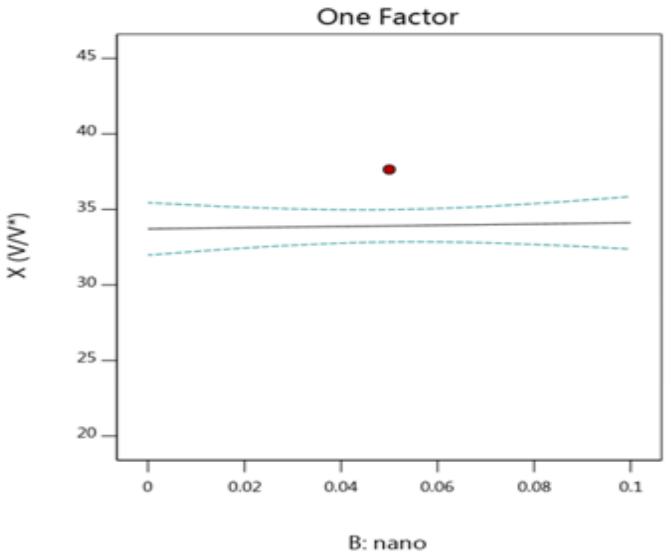

Diagram 2. Effect of nanoparticles on solubility

Diagram (2), as in diagram (1), shows the effect of nanoparticles on CO_2 solubility at 10 bar pressure and 15 wt% solvent. This is negligible compared to the other two parameters (pressure and solvent).

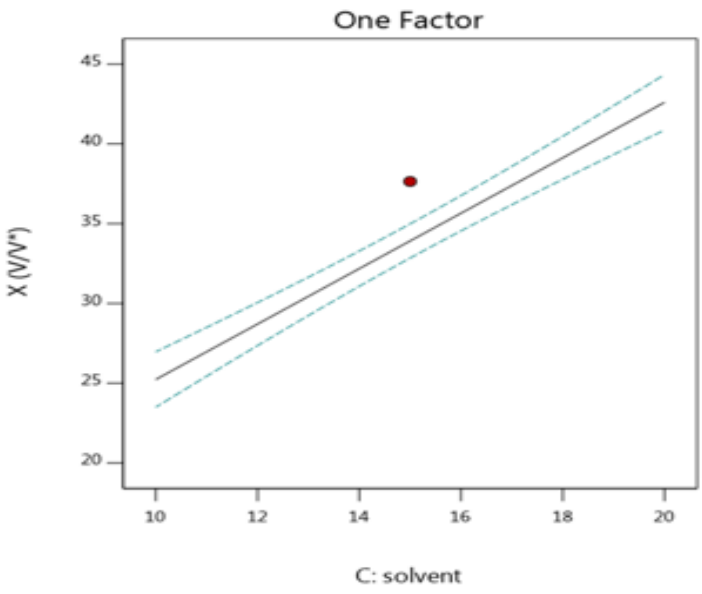

Diagram 3. Effect of amine solution on solubility

Diagram (3) shows the influence of the solvent on carbon dioxide solubility at 10 bar pressure

and 0.05 wt% nanoparticle concentration. It is found that the solvent has a tremendous effect on the solubility of CO_2 compared to the other two parameters (pressure and nanoparticles).

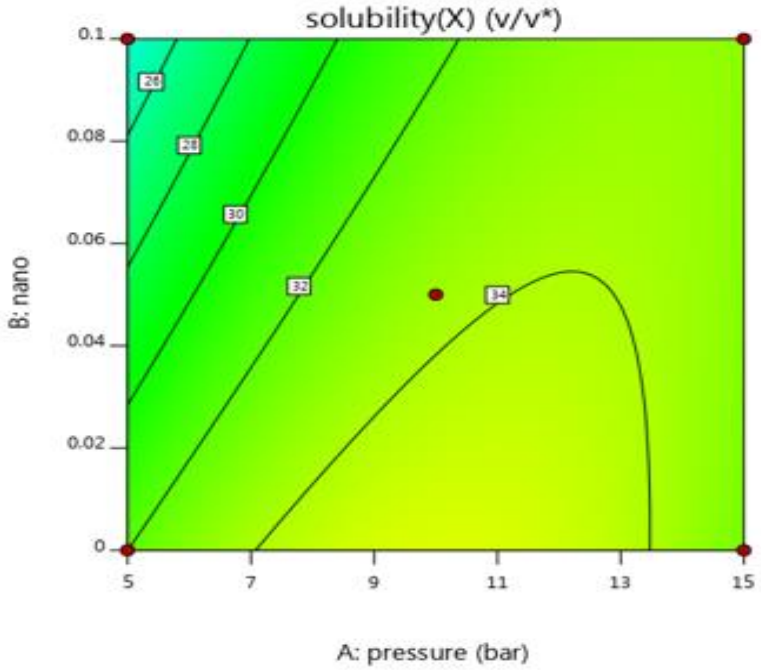

Diagram 4. Simultaneous effect of pressure and nanoparticles on solubility

Diagram (4) shows that by choosing a constant concentration of 15 wt% solvent, pressure and nanoparticles have no significant effect on solubility.

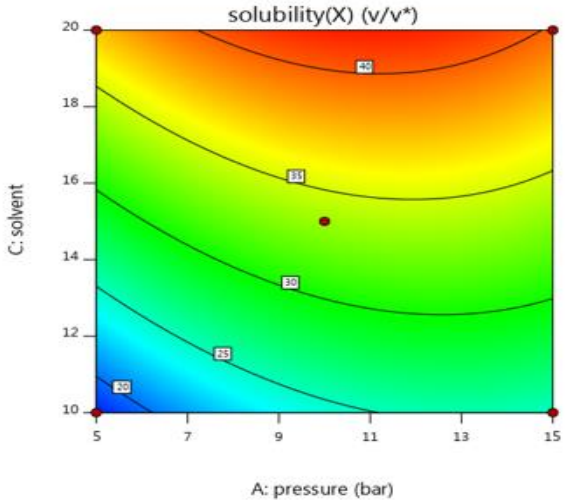

Diagram 5. Simultaneous effect of pressure and solvent on solubility

Diagram (5) shows that for nanoparticles with a concentration of 0.05 wt.%, The maximum solubility effect at solvent concentrations exceeds 15 wt% and a pressure of 5 to 15 bar.

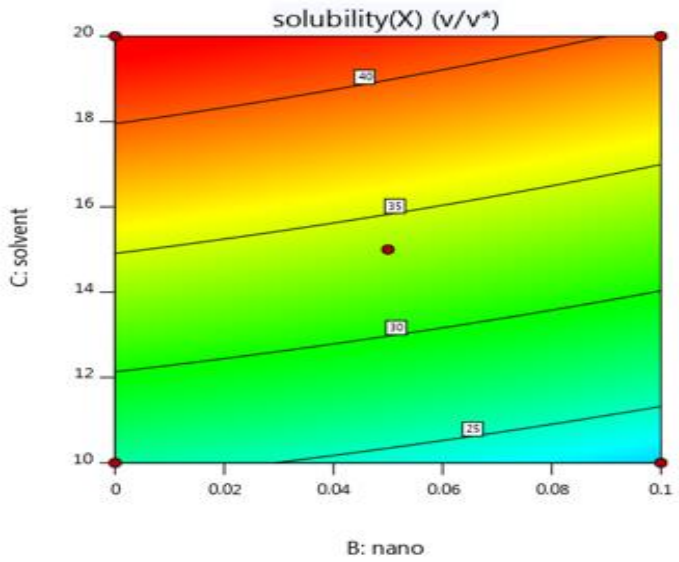

Diagram 6. Simultaneous effect of solution and Nano-particle on solubility

Diagram (6) shows that at 10 bar pressure, the highest solubility percentage occurs for nanoparticle concentrations between 0 and 0.1 and the solvent exceeding 15 wt.%.

Conclusion

In this study, the solubility of carbon dioxide (CO_2) in diethyl ethanolamine (DEEA) with and without the presence of calcium carbonate nanoparticles ($CaCO_3$) has been investigated, the results of which are as follows:

All experiments were performed at constant temperature, so the effect of temperature was included in any of the results. Experiments were generally performed in 13 steps at three different pressures 5, 10 and 15 bar to investigate the solubility of carbon dioxide in diethyl ethanolamine solution at concentrations of 10, 15 and 20 wt% in the presence and absence of nanoparticles. Calcium carbonate was obtained at 0.05 and 0.1 wt%. The results showed that at constant pressure, with increasing concentration of DEEA solution, carbon dioxide solubility increased but increase in calcium carbonate nanoparticles had no significant effect on solubility. When the concentration of DEEA solution is constant, CO_2 solubility increases with increasing

system pressure. On the other hand, according to the analysis of the design expert-11 software diagrams, it is deduced that the DEEA solution is the most effective solubility parameter for solubility.

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