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CHAPTER 1: INTRODUCTION

1. PROJECT BACKGROUND

1.1 Background Study

Environmental issues due to emissions of pollutants from combustion of fossil fuels have become global problems, including air toxics and greenhouse gases (GHG). Among these GHG, CO₂ is the largest contributor in regard of its amount present in the atmosphere contributing to 60 % of global warming effects^[1]. Scientists theorize that an increase in these greenhouse gases will translate into increased temperatures around the globe, which would result in many disastrous environmental effects. In fact, the Intergovernmental Panel on Climate Change (IPCC) predicts in its *'Fourth Assessment Report'* released in 2007 that during the 21st century, global average temperatures are expected to rise by between 2.0 and 11.5 °C Fahrenheit. A Fifth Assessment Report is expected to be released sometime between 2010 and 2015^[2]. Therefore, CO₂ needs to be separated and captured from the flue gases, natural gases, refinery off-gases, synthesis gas and other industrial gases of such point sources before direct sequestration.

Removal of acid gases is an important industrial operation. As we have known, there are various technologies being used to separate CO₂ from the flue gas e.g., chemical absorption, physical absorption, cryogenic methods, membrane separation, and biological fixation^[3]. Chemical absorption process is generally recognized as the most effective technology^[4]. Due to their active nature, acidic gases may be absorbed from a gas stream by a number of different chemical or physical absorbents. When CO₂ are present in a gas stream, the most commonly used absorbents are aqueous solutions of a single or mixed alkanolamine.

Alkanolamine solutions are one of the methods and widely used for the removal of acid gases such as CO₂ and H₂S from process streams containing these components in the industries. The technique has been proven to be reliable and has found wide application in many chemical industries such as ammonia production, coal gasification and natural gas processing. Alkanolamines are broadly classified into primary, secondary and tertiary as well as a new class of amines known as sterically hindered amines that has been introduced a few years ago. Examples of these amines are monoethanolamine (MEA), diethanolamine (DEA), methyldiethanolamine (MDEA) and amino-methylpropane (AMP) respectively.

The most extensively studied CO₂ absorption system is monoethanolamine (MEA) absorption process ^[5]. There are some disadvantages of using the MEA absorption system which are include: (1) low CO₂ loading capacity; (2) high equipment corrosion rate; (3) amine degradation by SO₂, NO₂, HCl, HF, and oxygen which include a high absorbent makeup rate; (4) high energy consumption during high temperature absorbent regeneration. While for the secondary amine (DEA), the low vapor pressure of DEA makes it suitable for low pressure operations, as vaporization losses are quite negligible. Generally, DEA solution is less corrosive when compared to MEA solutions. In view of this, DEA based blend appear to be potential solvents for CO₂ absorption in gas treating system ^[1].

Both primary and secondary amines generally exhibit low CO₂ loadings but with a high rate of absorption. Primary and secondary amines react rapidly with CO₂ to form carbamate with a stoichiometric loading of 0.5 mol CO₂/mol amine. In contrast, tertiary amines show the opposite behavior. For the tertiary amine MDEA, the CO₂ loading approaches a value of 1.0 mol CO₂/mol amine due to their not forming carbamates ^[1]. However, sterically hindered amines have been known to exhibit a high loading with a high absorption rate ^[6]. Mixed amines can bring about considerable improvement in gas absorption and great

savings in energy requirement for regeneration, e.g., mixture of primary (MEA) or secondary (DEA) alkanolamine with a tertiary alkanolamine(MDEA).

Therefore, as alkanolamines which classified into primary, secondary, tertiary and sterically hindered amines have their own advantages in term of CO₂ loading and absorption rate, kinetics or solubility study become a prime concern in order to increase the effectiveness of the performance amine based solvent to capture CO₂ in the gas stream.

1.2 Problem Statement

The low vapor pressure of DEA makes it suitable for low pressure operation as vaporization losses are quite negligible. Generally, DEA solutions are less corrosive when compared to MEA solutions ^[6]. Recently, piperazine (PZ) has been used as a good promoter because of its rapid formation of carbamates with CO₂ when mixed with MDEA. Piperazine (PZ) could potentially be high-efficiency solvents for the industrial CO₂ removal process; however, the solubility of CO₂ in aqueous blends of DEA with PZ have not been extensively investigated so far and very scarce in the literature. The solubility of CO₂ for total amine concentrations and mole fraction of PZ to total amine ranging from 2.0 to 3.0M and 0.01 to 0.02 were reported at temperatures and CO₂ partial pressures ranging from (303.14 to 353.14)K and (10.133 to 20.265)kPa^[1]. Other solubility data of DEA/PZ aqueous solutions have not been reported in the literature. Therefore, the objective of this research is to study experimentally the solubility of CO₂ in aqueous DEA/PZ solutions at temperature of 30°C, 50°C and 70°C and at partial pressure of CO₂ between 200-1000kPa. The blended amine aqueous solutions chosen for study are 20wt%DEA, 40wt% DEA, 5wt % PZ and 10wt% PZ.

1.3 Objectives

The objectives of this study are:

1. To determine the effect of PZ to the CO₂ solubility.
2. To study the effect of temperature and pressure to CO₂ solubility.
3. To determine the physical properties of blend amine in term of density, viscosity and refractive index.

1.4 Scope of study

Before beginning the test for solubility, the physical properties (density, viscosity, and refractive Index) of difference concentrations of the aqueous amine blends were determined. The concentrations of the aqueous amine are 20wt% DEA, 40wt% DEA, and 20wt% DEA+5wt% PZ, 20wt% DEA+10wt% PZ, 40wt% DEA+5wt% PZ, 40wt% DEA+10wt% PZ. The solubility of CO₂ in aqueous blends of diethanolamine (DEA) and piperazine (PZ), was measured for temperatures and CO₂ partial pressures ranging from (303.14 to 343.14) K and (200 to 1500) kPa, respectively. Measurements were made by cell solubility equipment. The solubility of carbon dioxide in aqueous solutions is reported as functions of partial pressures of carbon dioxide at the temperatures studied.

1.5 Relevancy of the Project

CO₂ removal becomes a mandatory in industrial operation when more technologies has been developed and applied in order to decrease the CO₂ emission to the atmosphere. Impacts of amine solvent on human health and the environment have, however, received considerably less attention^[8]. The results which will be presented in this paper can expose great potential of blended amine base solvent that might lead to a better approach for development of

advanced technologies in CO₂ capture with the new blended amine solvent can operate at much higher concentrations with low corrosion potential.

CHAPTER 2: LITERATURE REVIEW

2.1 Absorption by Alkanolamines

A wide variety of separation techniques involves the removal of vapor-phase impurities from gas stream including permeation through membrane, absorption into a liquid, condensation, chemical conversion to another compound and adsorption on a solid^[3]. One effective approach to remove CO₂ from the gas stream is by absorption of CO₂ in aqueous solution of alkanolamine, couples physical absorption with chemical reactions where both kinetics and thermodynamic equilibrium may play important roles in determining the ultimate gas loading^[3].

Solutions of alkanolamines are an industrially important class of compounds used in the natural gas, petroleum chemical plants, and ammonia industries for the removal of CO₂ and H₂S from gas streams. A wide variety of alkanolamines such as monoethanolamine (MEA), diethanolamine (DEA), diisopropanolamine (DIPA), *N*-methyldiethanolamine (MDEA) have been used industrially for a number of years^[9]. A recent advancement in gas treating technology is the application of sterically hindered amines which offer absorption capacity, absorption rate, selectivity, and degradation resistance advantages over conventional amines for CO₂ removal from gases^[10]. 2-amino-2-methyl-1-propanol (AMP) and 2-piperidineethanol (2-PE) are two of the sterically hindered amines.

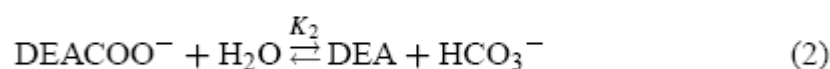
2.2 Theory

An equilibrium solution of CO₂ in aqueous solution of alkanolamine is governed by the following set of equations ^[1]:

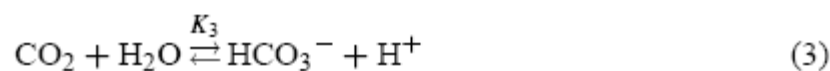
Dissociation of protonated amine:



Formation of carbamate:



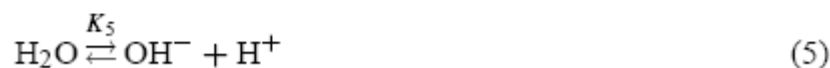
Dissociation of carbon dioxide:



Dissociation of bicarbonate ion:



Ionization of water:



The equilibrium constants for the above equations are expressed as follows:

$$K_1 = \frac{[\text{DEA}][\text{H}^+]_e \gamma_{\text{DEA}} \gamma_{\text{H}^+}}{[\text{DEAH}^+]_e \gamma_{\text{DEAH}^+}} \quad (6)$$

$$K_2 = \frac{[\text{DEACOO}^-]_e [\text{H}^+]_e \gamma_{\text{DEACOO}^-} \gamma_{\text{H}^+}}{[\text{DEA}]_e [\text{CO}_2]_e \gamma_{\text{DEA}} \gamma_{\text{CO}_2}} \quad (7)$$

$$K_3 = \frac{[\text{HCO}_3^-]_e [\text{H}^+]_e \gamma_{\text{HCO}_3^-} \gamma_{\text{H}^+}}{[\text{CO}_2]_e \gamma_{\text{CO}_2}} \quad (8)$$

$$K_4 = \frac{[\text{CO}_3^{2-}]_e [\text{H}^+]_e \gamma_{\text{CO}_3^{2-}} \gamma_{\text{H}^+}}{[\text{HCO}_3^-]_e \gamma_{\text{HCO}_3^-}} \quad (9)$$

$$K_5 = \frac{[\text{OH}^-]_e [\text{H}^+]_e}{a_{\text{H}_2\text{O}}} \gamma_{\text{OH}^-} \gamma_{\text{H}^+} \quad (10)$$

Where $[J]$ is the concentration of the various species, and γ_i is the activity coefficient of each species. In addition to the above equations, the following set of conditions must also be satisfied ^[1].

Amine balance:

$$[\text{DEA}]_t = [\text{DEA}]_e + [\text{DEAH}^+]_e + [\text{DEACOO}^-]_e \quad (11)$$

CO₂ balance:

$$\alpha[\text{DEA}]_t = [\text{HCO}_3^-]_e + [\text{DEACOO}^-]_e + [\text{CO}_3^{2-}]_e + \frac{P_{\text{CO}_2}}{H_{\text{CO}_2}} \quad (12)$$

Charge balance:

$$[\text{DEAH}^+]_e = [\text{HCO}_3^-]_e + [\text{DEACOO}^-]_e + 2[\text{CO}_3^{2-}]_e \quad (13)$$

Where α is the gas loading. The concentration of carbon dioxide in the liquid phase can be estimated from Henry's law, i.e.^[1].

$$P_{\text{CO}_2} = H_{\text{CO}_2}[\text{CO}_2]$$

Where P_{CO_2} is the CO₂ partial pressure, kPa, H_{CO_2} is the Henry's law constant, kPa.m³/kmol, $[\text{CO}_2]$ is the concentration of CO₂, kmol/m³.

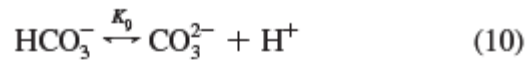
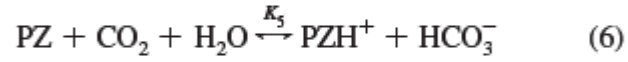
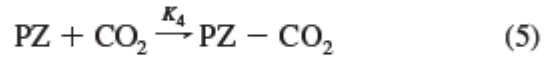
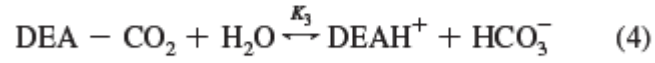
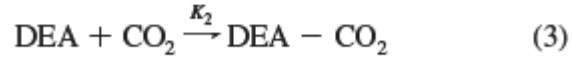
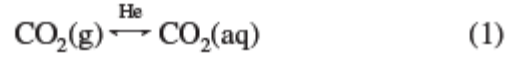
2.3 Piperazine as a Promoter

Recently, there is an interest in employing the reaction rate accelerator e.g., piperazine (PZ) in the aqueous alkanolamine solution. PZ is a cyclic, diamine that has previously been studied as a promoter for amine systems such as MDEA/PZ or MEA/PZ blends to improve CO₂ mass transfer rates and it is reported that PZ is more effective than the conventional activators ^[11]. The concentration of PZ when used as a promoter was low, between 0.5 and 2.5 M PZ, because PZ is not highly soluble. Given the nature and magnitude of absorption/stripping systems, any possibility of precipitation ruled out PZ for use at concentrations above its room temperature solubility ^[16].

Additionally, the boiling point of PZ (146.5 °C) is lower than that of MEA (170°C), indicating the possibility for higher volatility. Recent work has indicated that the volatility of PZ is comparable to that of MEA due to the non-ideality of PZ in solution ^[12]. Increasing the concentration of PZ in solution allows for increased solvent capacity and faster CO₂ absorption rates. PZ has been studied as a solvent for absorption/stripping systems for the removal of CO₂ from the flue gas of coal-fired power plants. The current work examines solid solubility, oxidation, thermal degradation, and CO₂ solubility of concentrated aqueous PZ solutions. Additionally, extensive work on the mass transfer of CO₂ into PZ is reported. Finally, preliminary modeling work indicates that stripper performance with a concentrated PZ solvent is slightly enhanced compared to pure MEA systems ^[16].

2.3.1 CO₂ Solubility Model

The chemical reaction equilibria and gas-liquid phase equilibria for the (CO₂ +DEA + PZ + H₂O) system are coexistent. When CO₂ is absorbed into an aqueous solution of PZ mixed with DEA, the following reaction may occur ^[11]:-



$$p_{\text{CO}_2} = H_{\text{e}} C_{\text{CO}_2} \quad (12)$$

$$K_1 = C_{\text{DEAH}^+} / C_{\text{DEA}} C_{\text{H}^+} \quad (13)$$

$$K_3 = C_{\text{DEAH}^+} C_{\text{HCO}_3^-} / C_{\text{DEA-CO}_2} C_{\text{H}_2\text{O}} \quad (14)$$

$$K_5 = C_{\text{PZH}^+} C_{\text{HCO}_3^-} / C_{\text{PZ-CO}_2} C_{\text{H}_2\text{O}} \quad (15)$$

$$K_6 = C_{\text{PZCOO}^-} C_{\text{H}^+} / C_{\text{PZ}} C_{\text{CO}_2} \quad (16)$$

$$K_7 = C_{\text{PZH}^+} / C_{\text{PZ}} C_{\text{H}^+} \quad (17)$$

$$K_8 = C_{\text{DEA-CO}_2} C_{\text{PZ}} / C_{\text{PZ-CO}_2} C_{\text{DEA}} \quad (18)$$

$$K_9 = C_{\text{CO}_3^{2-}} C_{\text{H}^+} / C_{\text{HCO}_3^-} \quad (19)$$

$$K_{10} = C_{\text{H}^+} C_{\text{OH}^-} / C_{\text{H}_2\text{O}} \quad (20)$$

Where C stands for amount concentration of ions and molecular species, K_1 to K_{10} and H are concentration equilibrium constants and Henry's constant respectively. In addition, the following mass and charge balances governing the reacting species can be formed ^[1];-

$$C_{\text{DEA}}^0 = C_{\text{DEA}} + C_{\text{DEAH}^+} \quad (21)$$

$$C_{\text{PZ}}^0 = C_{\text{PZ}} + C_{\text{PZH}^+} + C_{\text{PZCOO}^-} \quad (22)$$

$$C_{\text{HCO}_3^-} + C_{\text{CO}_3^{2-}} + C_{\text{CO}_2} + C_{\text{PZCOO}^-} = \alpha_{\text{CO}_2} (C_{\text{DEA}}^0 + C_{\text{PZ}}^0) \quad (23)$$

$$C_{\text{DEAH}^+} + C_{\text{PZH}^+} + C_{\text{H}^+} = C_{\text{OH}^-} + C_{\text{HCO}_3^-} + 2C_{\text{CO}_3^{2-}} + C_{\text{PZCOO}^-} \quad (24)$$

Where C^0 and α_{CO_2} are the initial concentration of molecular species and solubility of CO_2 in the liquid phase, respectively. Defining α_{D} as the ratio of DEAH^+ to DEA, α_{P1} as that of PZCOO^- to PZ, and α_{P2} as that of PZH^+ to PZ in the solution

$$\alpha_{\text{D}} = C_{\text{DEAH}^+} / C_{\text{DEA}}^0 \quad (25)$$

$$\alpha_{\text{P1}} = C_{\text{PZCOO}^-} / C_{\text{PZ}}^0 \quad (26)$$

$$\alpha_{\text{P2}} = C_{\text{PZH}^+} / C_{\text{PZ}}^0 \quad (27)$$

From equation 16 and 17, a relationship between PZCOO^- and PZH^+ is obtained

$$C_{\text{CO}_2} = \alpha_{\text{P1}} \alpha_{\text{P2}} / ((1 - \alpha_{\text{P1}} - \alpha_{\text{P2}})^2 K_6 K_7) \quad (28)$$

From equation 14, 15, and 18, the distribution between DEA and PZ is given by

$$K_1 / K_7 = (K_3 K_8 / K_5) = ((1 - \alpha_{\text{P1}} - \alpha_{\text{P2}}) \alpha_{\text{D}}) / (\alpha_{\text{P2}} (1 - \alpha_{\text{D}})) \quad (29)$$

2.4 Effect of Different Concentration of PZ, Temperature and Partial Pressure on CO_2 Solubility

The different concentration of PZ in DEA blend solution, temperature and partial pressure of CO_2 have a large effect on CO_2 solubility. From the previous study, from Figure 1 it is clear that CO_2 solubility in amine blend exhibits a decreasing nature with total amine concentration of blend. The effect of total amine concentration is less pronounced at a high concentration range. A comparison of CO_2 solubility in aqueous DEA solution is also shown at

complete concentration range with data of ^[1]. It is seen from Figure 2 that solubility of CO₂ increases as the partial pressure of CO₂ in the inlet gas stream is increased at a particular temperature. The effect of partial pressure of CO₂ in the inlet gas stream is almost the same at all molar ratios of piperazine in total amine blend. From Figure 3, as the temperature increases, the CO₂ solubility decreases at a particular total amine concentration. With increasing molar ratio of piperazine in total amine blend, the CO₂ solubility increases at a particular total concentration of amine blend in Figure 4.

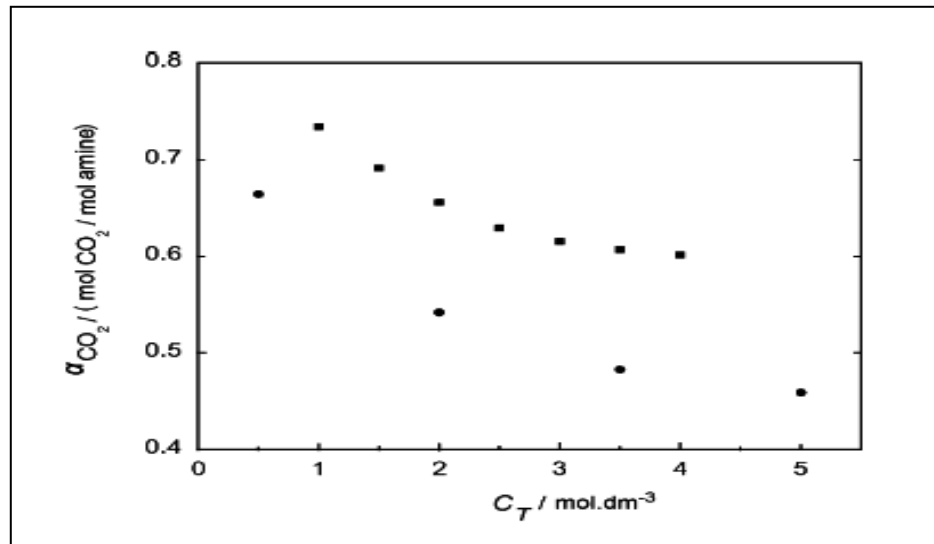


Figure 1: Effect of total concentration of amine blend C_T on CO₂ loading α_{CO_2} at $T = 313.14 \text{ K}$, $p_{\text{CO}_2} = 15.199 \text{ kPa}$, and mole ratio of PZ in total amine $X_1 = 0.2$ of \blacksquare , (DEA + PZ) blend, present study; \bullet aq DEA, ^[13]

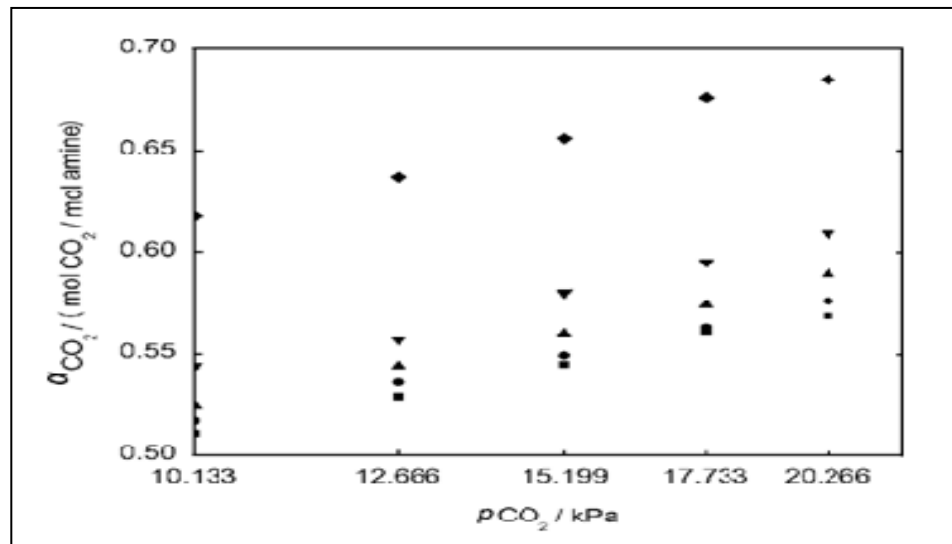


Figure 2: Effect of CO₂ partial pressure in inlet gas stream p_{CO_2} on CO₂ loading α_{CO_2} with mole ratio of PZ in total amine X_1 of \blacksquare , 0.01; \bullet , 0.02; \blacktriangle , 0.05; \blacktriangledown , 0.10; \blacklozenge , 0.20 in (DEA + PZ) blend at T 313.14 K and total concentration of amine blend C_T) 2.0 mol · dm⁻³.

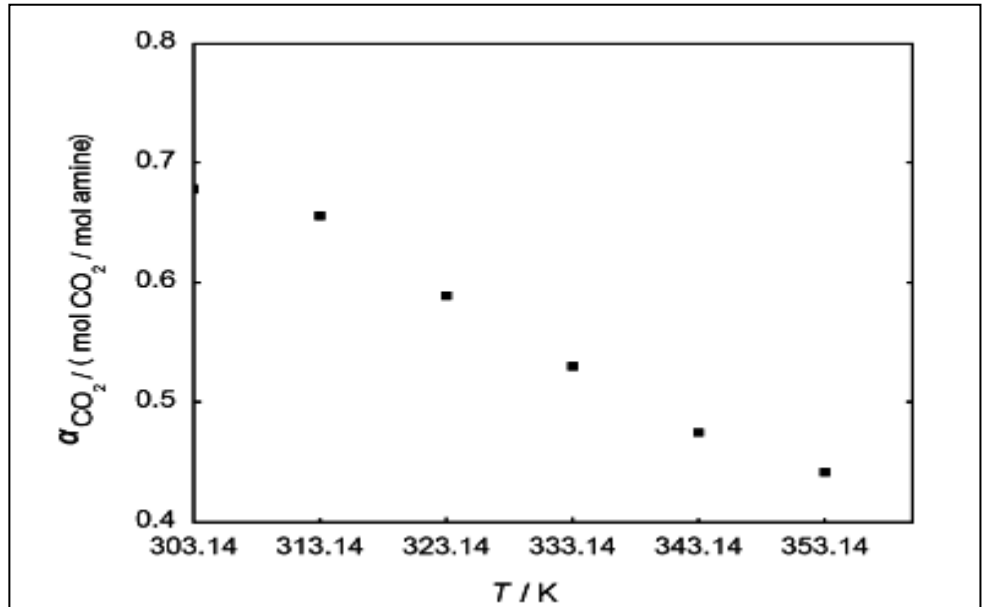


Figure 3: Effect of temperature T on CO_2 loading α_{CO_2} in (DEA + PZ) blend at $p_{CO_2} = 15.199$ kPa, total concentration of amine blend $C_T = 2.0$ mol \cdot dm⁻³, and mole ratio of PZ in total amine $X_1 = 0.2$.

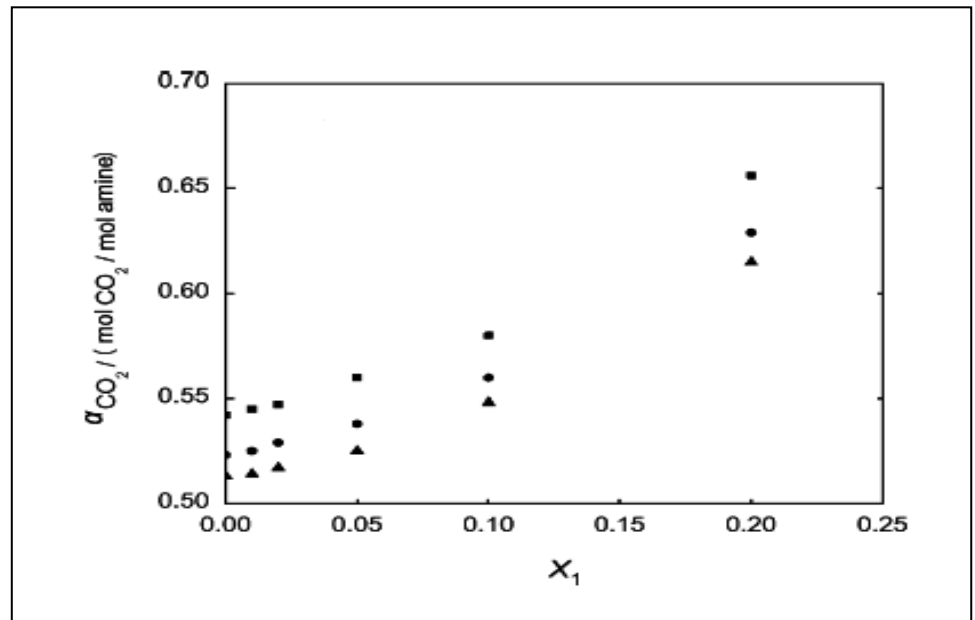


Figure 4: CO_2 loading α_{CO_2} with different mole ratios of PZ in total amine X_1 at $T = 313.14$ K and $p_{CO_2} = 15.199$ kPa for total concentration of amine blend C_T of \bullet 2.0 mol \cdot dm⁻³; \blacktriangle 5 mol \cdot dm⁻³; \blacksquare 3.0 mol \cdot dm⁻³.

CHAPTER 3: METHODOLOGY

3.1 Research Methodology

The research methodology is divided into three categories: Materials, Experimental Work and Theoretical Work.

3.1.1 Materials

3.1.1.1 Chemicals

PZ with stated purity of 99.9 % (GC, area %), and DEA with purity of 99.5 % (GC, area %), were supplied by Merck company and were used without further purification. The aqueous PZ and aqueous (DEA + PZ) solutions were prepared gravimetrically with a precision of 0.0001 g using an analytical balance (Mettler Toledo model AS120S). The possible uncertainty in calculating mole fraction and mass fraction of aqueous solutions was estimated to be around ± 0.001 and ± 0.0001 , respectively. All measurements for each sample were performed in duplicate, and the average values are reported.

3.1.1.2 Equipment

High Pressure Gas Solubility Cell

3.1.2 Experimental Work

3.1.2.1 Solubility Measurement

In order to make CO₂ solubility measurements over the DEA/PZ aqueous solutions at partial pressures of CO₂, from 200-1500 kPa, High pressure gas solubility cell is used. Approximately 5 mL of the solvent was fed by gravity to the equilibrium cell. The apparatus was then purged with CO₂ to

remove traces of oxygen and was brought to the desired temperature. The partial pressure of CO₂ was adjusted to an amount indicated by the total pressure of the system in the range of 200-1000 kPa. The temperature of the cell was controlled by a temperature controller made by Autoclave Engineers. When the total pressure of the cell does not change for 1 h, the equilibrium is assumed to have been reached. Usually it would take 4 h for the system to attain equilibrium. At equilibrium, the reading of the pressure drop will be taken for calculation of solubility purpose. The CO₂ partial pressure was obtained by subtracting the reading for pressure drop from the total pressure of the system.



Figure 5: High Pressure Gas Solubility Cell

3.1.2.2 Density Measurement

A digital vibrating glass U-tube densitometer (DMA5000, Anton-Paar) was used for density measurements with an accuracy of $\pm 0.003 \text{ kg} \cdot \text{m}^{-3}$ at temperatures (303.15 to 343.15) K. The temperature accuracy of $\pm 0.02 \text{ K}$ (traceable to the ITS-90 protocol) was maintained with a built-in platinum resistance thermometer. The experimental uncertainty for temperature and density measurements is estimated to be $\pm 0.03 \text{ K}$ and $\pm 0.005 \text{ kg} \cdot \text{m}^{-3}$, respectively. The densitometer was calibrated using Millipore quality water samples before and after all density measurements^[7].

3.1.2.3 Viscosity Measurement

The kinematic viscosity of the samples was measured at temperatures (303.15 to 343.15) K using calibrated Ubbelohde viscometers of appropriate sizes that were immersed in a thermostatic bath (Tamson, TVB445). The calibrated Ubbelohde viscometers were further verified with the standard solvents of known viscosity (provided by the equipment supplier) and found to be in good agreement. The bath temperature was regulated with a Pt-100 temperature probe with an accuracy of $\pm 0.02 \text{ K}$. The dynamic viscosity of the samples was calculated using kinematic viscosity and corresponding density values with an uncertainty of $\pm 0.3 \%$. The experimental viscosity at corresponding temperatures was measured with an uncertainty of $\pm 0.04 \text{ mPa} \cdot \text{s}$ and $\pm 0.04 \text{ K}$, respectively^[18].

3.1.2.4 Refractive Index

The refractive index(RI) of the samples was determined using a programmable digital refractometer (Atago, RX-5000 alpha) with a measuring accuracy of $\pm 4 \cdot 10^{-5}$. The refractometer was calibrated using Millipore quality water before each series of measurements and checked for ethanol (absolute, Fischer scientific) with purity 99.4 % and known refractive index of 1.36242. The refractive indices were measured at (303.15 to 343.15) K with a temperature control accuracy of ± 0.05 K. The experimental uncertainty for refractive index measurement at corresponding temperatures was found to be $\pm 3 \cdot 10^{-5}$ and ± 0.05 K, respectively^[7].

Table 1: Densities of ($\rho/\text{g}\cdot\text{cm}^{-3}$) of piperazine + water

T/K	100 (w_2)					
	1.74	ref 19	3.45	6.88	10.35	ref 19
298.15	0.99775	0.998287	0.99852	1.00018	1.00223	1.001285
303.15	0.99637		0.99708	0.99869	1.00064	
308.15	0.99474	0.995233	0.99543	0.99697	0.99884	0.998022
313.15	0.99291		0.99359	0.99507	0.99686	
318.15	0.99090	0.991382	0.99156	0.99299	0.99473	0.993991
323.15	0.98872		0.98935	0.99074	0.99239	
328.15	0.98637		0.98698	0.98833	0.98992	
333.15	0.98383		0.98446	0.98577	0.98730	

Table 2: Viscosities (η /mPa.s) of piperazine + water

T/K	(100 w_2)					
	1.74	ref 19	3.45	6.88	10.35	ref 19
298.15	0.87	0.86	0.94	1.08	1.29	1.28
303.15	0.78		0.85	0.96	1.18	
308.15	0.71		0.75	0.86	1.04	
313.15	0.68	0.69	0.69	0.78	0.90	
318.15	0.59		0.63	0.71	0.84	
323.15	0.54		0.57	0.65	0.78	0.81
328.15	0.50		0.52	0.58	0.68	
333.15	0.46	0.47	0.48	0.54	0.62	0.59

Table 3: Refractive Indices (n_D) of piperazine + water

T/K	(100 w_1)					
	1.74	ref 19	3.45	6.88	10.35	ref 19
298.15	1.33796		1.34183	1.34759	1.35307	
303.15	1.33706	1.33449	1.34024	1.34608	1.35203	1.34847
313.15	1.33604	1.33366	1.33892	1.34482	1.35071	1.34797
323.15	1.33476		1.33759	1.34336	1.34957	
333.15	1.33348		1.33577	1.34221	1.34829	

3.1.3 Theoretical Work

The solubility measurements presented here were carried out in a High Pressure Gas Solubility Cell. The reactor consists of a 300ml stainless steel cylindrical tank with an air-driven magnetically coupled stirrer on the top. There are valves for inlet of gas and liquid, and a connection to a vacuum pump. A thermocouple inserted in the cell measures the temperature to an accuracy of 0.1 K. The pressure is measured by a pressure transducer with an accuracy of 0.14 kPa.

Initially a weighed sample of approximately 5ml of liquid is sucked into reactor below.

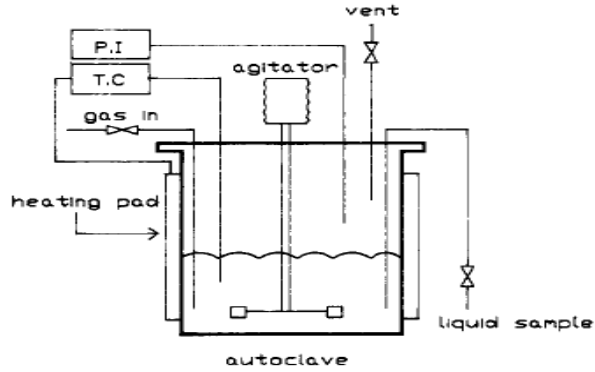


Figure 6: High Pressure vapor-liquid equilibrium apparatus

The temperature is then adjusted to the desired value through use of the external heating jackets. A vacuum is then pulled on the reactor so that the liquid exists under its own vapor pressure. This solution vapor pressure, P_v , is measured. A known quantity of CO_2 , n_{CO_2} , is transferred to the reactor from a gas container of known volume

$$n_{\text{CO}_2} = \frac{V_T}{RT_a} \left(\frac{P_1}{z_1} - \frac{P_2}{z_2} \right) \quad (1)$$

where V_T is the volume of the gas container, z_1 and z_2 are The compressibility factors corresponding to the initial pressure, P_1 , and the final pressure, P_2 , in the gas container before and after transferring the CO_2 , and T_a is the ambient temperature. After transferring the CO_2 to the reactor, the stirrer is turned on and equilibrium is attained in about 1hr. This equilibrium pressure $P_{\text{CO}_2} = (P_{T1} - P_v)$ is measured, and the moles of CO_2 remaining in the gas phase are determined from

$$n_{\text{CO}_2}^g = \frac{V_g P_{\text{CO}_2}}{z_{\text{CO}_2} RT} \quad (2)$$

The moles of CO₂ in the liquid are then determined from

$$n_{\text{CO}_2}^l = n_{\text{CO}_2} - n_{\text{CO}_2}^g \quad (3)$$

The CO₂ loading in the liquid phase is defined as

$$L_{\text{CO}_2} = \frac{n_{\text{CO}_2}^l}{n_{\text{Am}}} \quad (4)$$

where n_{Am} is the moles of MDEA in the liquid phase

$$n_{\text{Am}} = \frac{m_{\text{MDEA}} \rho V_1}{M_{\text{MDEA}}} \quad (5)$$

Where m_{MDEA} is the mass fraction of MDEA in the aqueous solution, ρ is the solution density, V_1 is the volume of liquid in cell, and M_{MDEA} is the molecular weight of MDEA ^[17].

3.2 GANTT CHART/ KEY MILESTONE

Timelines for FYP 2

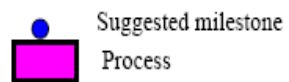
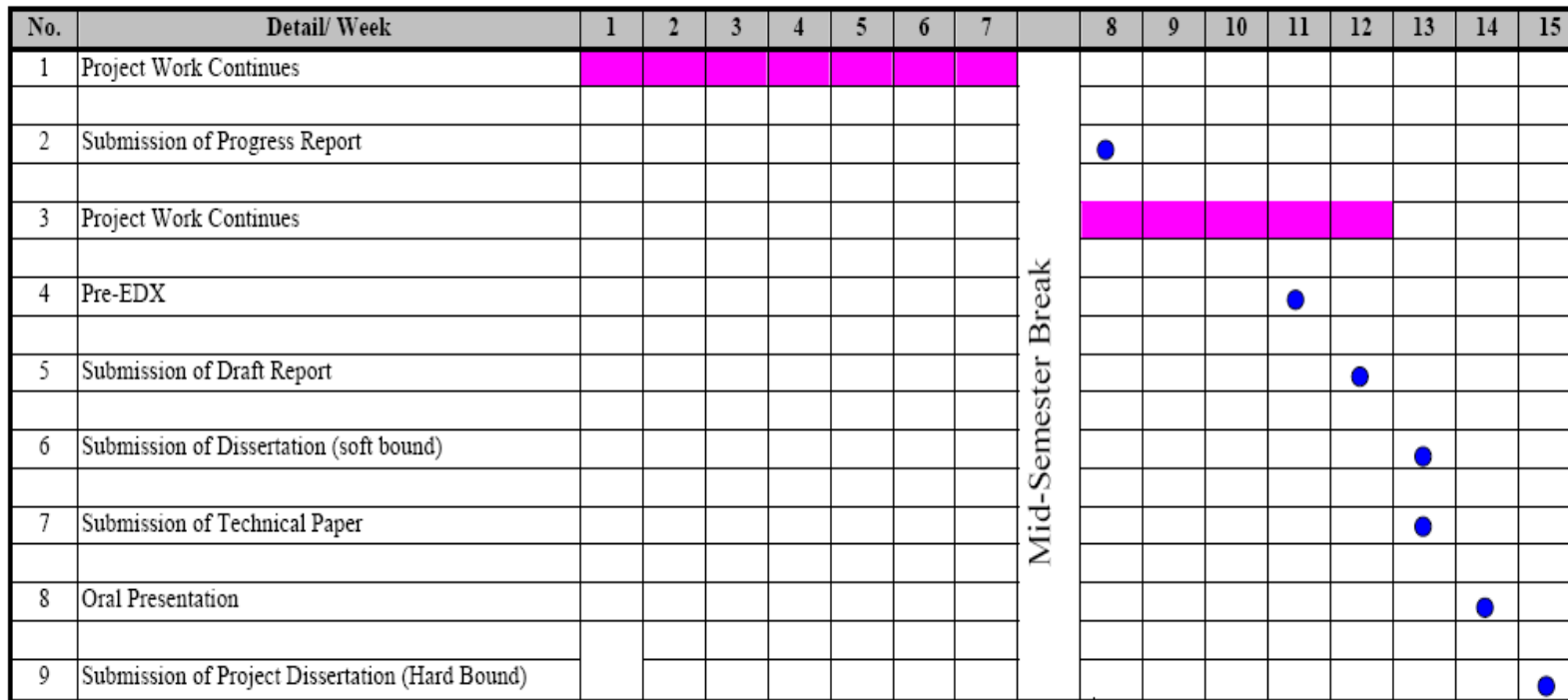


Figure 7: Gantt chart

CHAPTER 4: RESULT AND DISCUSSION

4.1 Result

4.1.1 Solubility Measurement Result

Table 4: Solubility of CO₂ in aqueous DEA/PZ at 303.14K

P(bar)	20wt%DEA	20wt%DEA+ 5wt%PZ	20wt%DEA+ 10wt%PZ	40wt%DEA	40wt%DEA+ 5wt%PZ	40wt%DEA+ 10wt%PZ
2	0.0868	0.0122	0.0136	0.0331	0.0714	0.0924
6	0.4083	0.7342	0.8604	0.3955	0.5744	0.6055
10	0.9040	1.5581	1.5087	0.7610	0.7008	0.8654

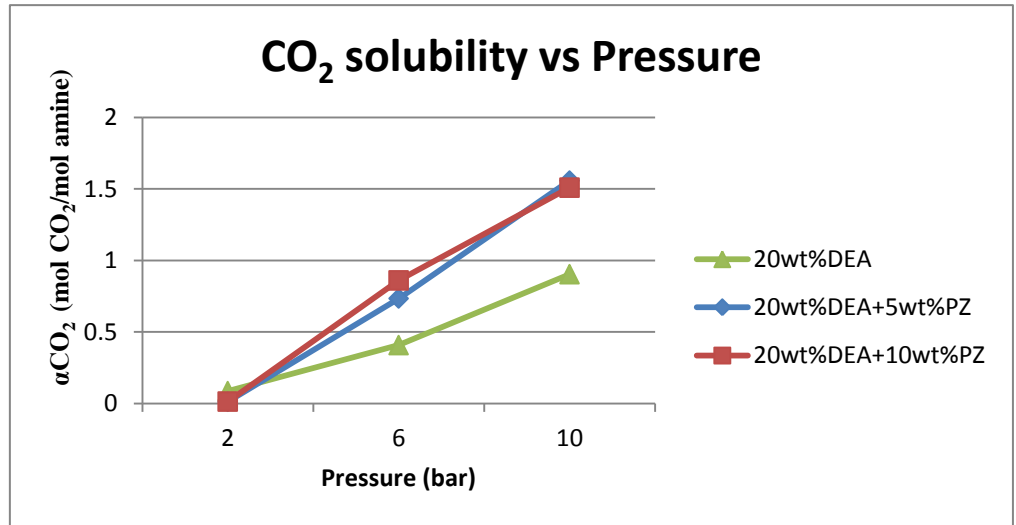


Figure 8: CO₂ loading α_{CO_2} with different mole ratios of PZ at $T = 303.14$ K and $p_{CO_2} = 200\text{kPa}, 600\text{kPa}, 1000\text{kPa}$ for total concentration of amine blend 2M

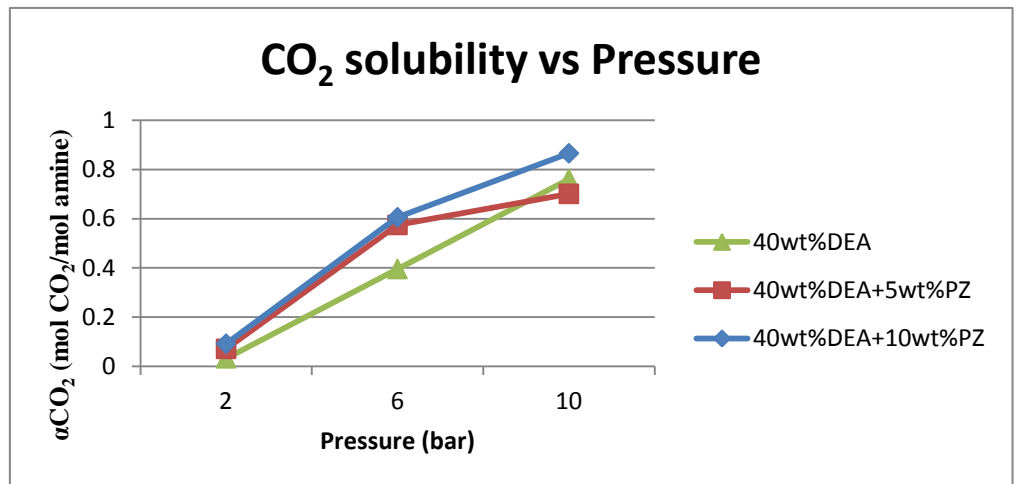


Figure 9: CO₂ loading α_{CO_2} with different mole ratios of PZ at $T = 303.14$ K and $p_{CO_2} = 200\text{kPa}, 600\text{kPa}, 1000\text{kPa}$ for total concentration of amine blend 4M

Table 5: Solubility of CO₂ in aqueous DEA/PZ at 323.14K

P(bar)	20wt%DEA	20wt%DEA+5wt%PZ	20wt%DEA+10wt%PZ	40wt%DEA	40wt%DEA+5wt%PZ	40wt%DEA+10wt%PZ
2	0.0978	0.1195	0.1265	0.0631	0.1424	0.0612
6	0.8941	0.6051	0.8416	0.5938	0.5801	0.5230
10	1.0308	1.3207	1.7263	0.7391	0.7725	0.9009

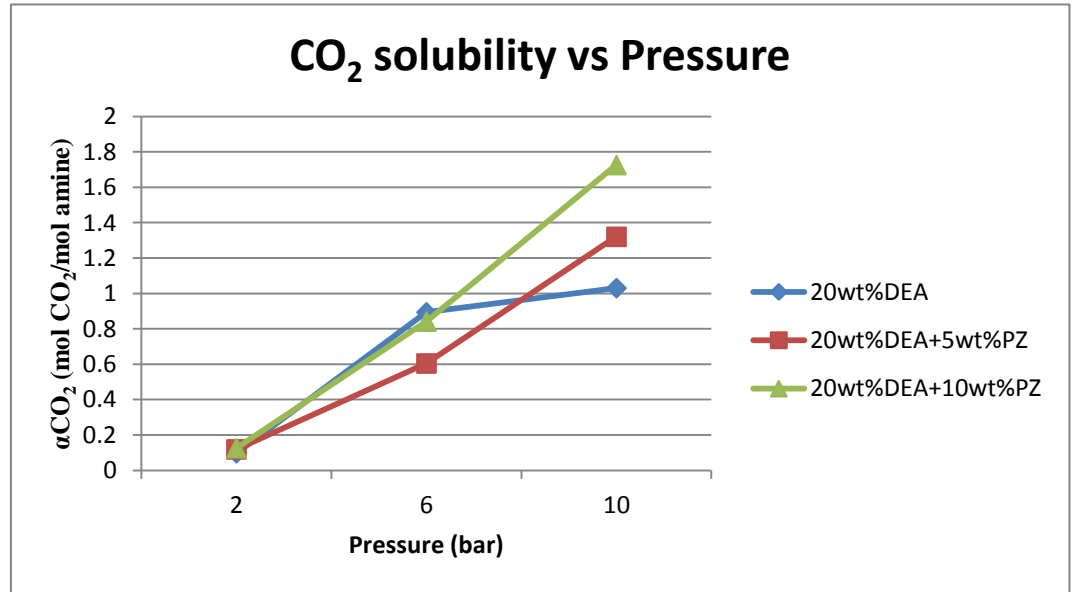


Figure 10: CO₂ loading α_{CO_2} with different mole ratios of PZ at $T = 323.14$ K and $p_{CO_2} = 200$ kPa, 600kPa, 1000kPa for total concentration of amine blend 2M

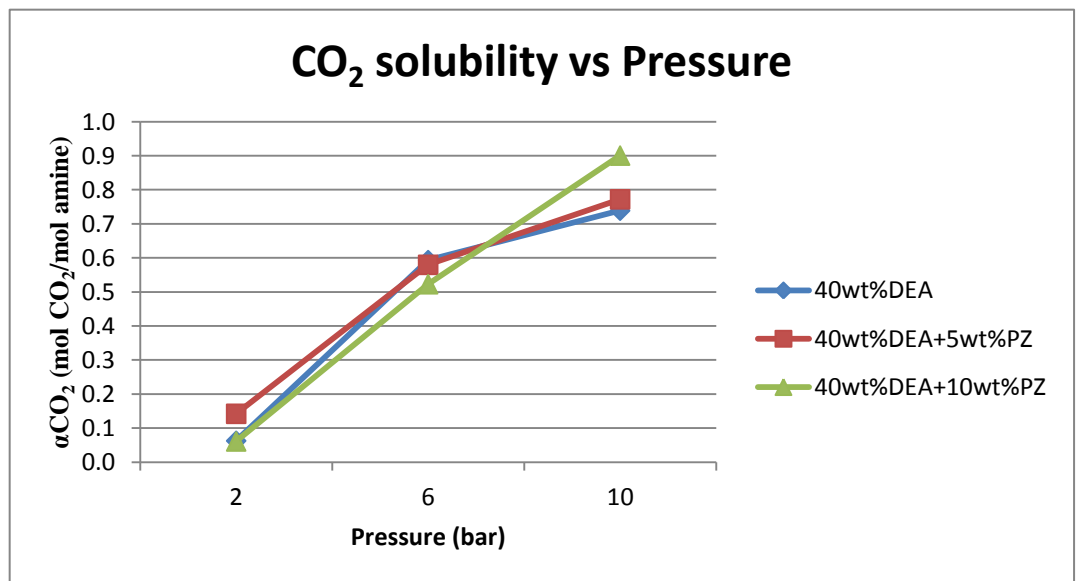


Figure 11: CO₂ loading α_{CO_2} with different mole ratios of PZ at $T = 323.14$ K and $p_{CO_2} = 200$ kPa, 600kPa, 1000kPa for total concentration of amine blend 4M

Table 6: Solubility of CO₂ in aqueous DEA/PZ at 343.14K

P(bar)	20wt%DEA	20wt%DEA+5wt%PZ	20wt%DEA+10wt%PZ	40wt%DEA	40wt%DEA+5wt%PZ	40wt%DEA+10wt%PZ
2	0.1311	0.0985	0.1229	0.1597	0.0627	0.0828
6	0.6241	0.8317	0.7488	0.5247	0.4308	0.6739
10	0.8176	1.4248	1.7334	0.7031	0.8853	1.0267

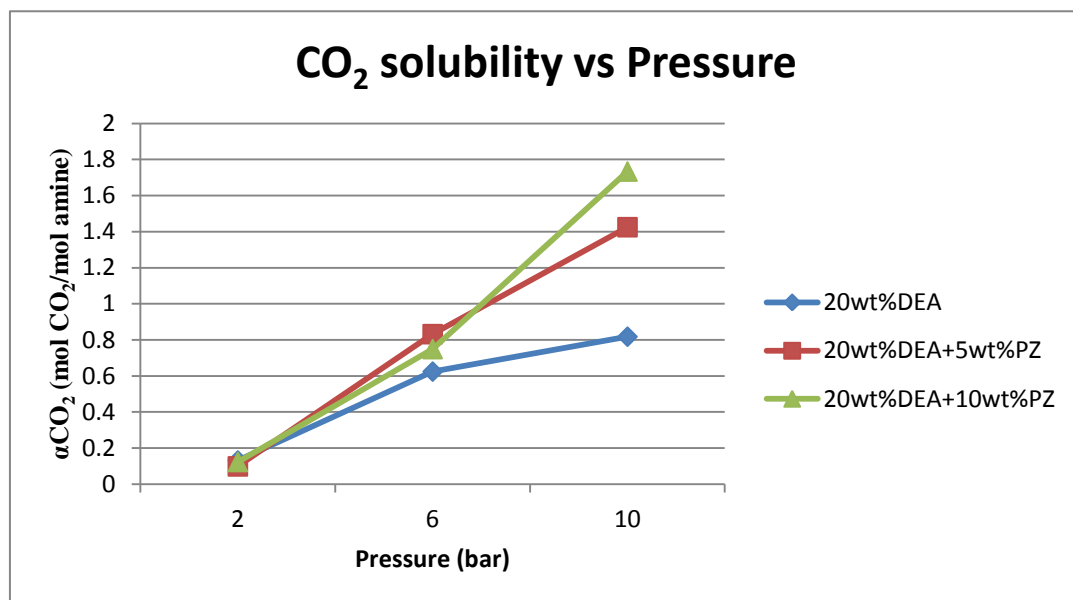


Figure 12: CO₂ loading α_{CO_2} with different mole ratios of PZ at $T = 343.14$ K and $p_{CO_2} = 200$ kPa, 600kPa, 1000kPa for total concentration of amine blend 2M

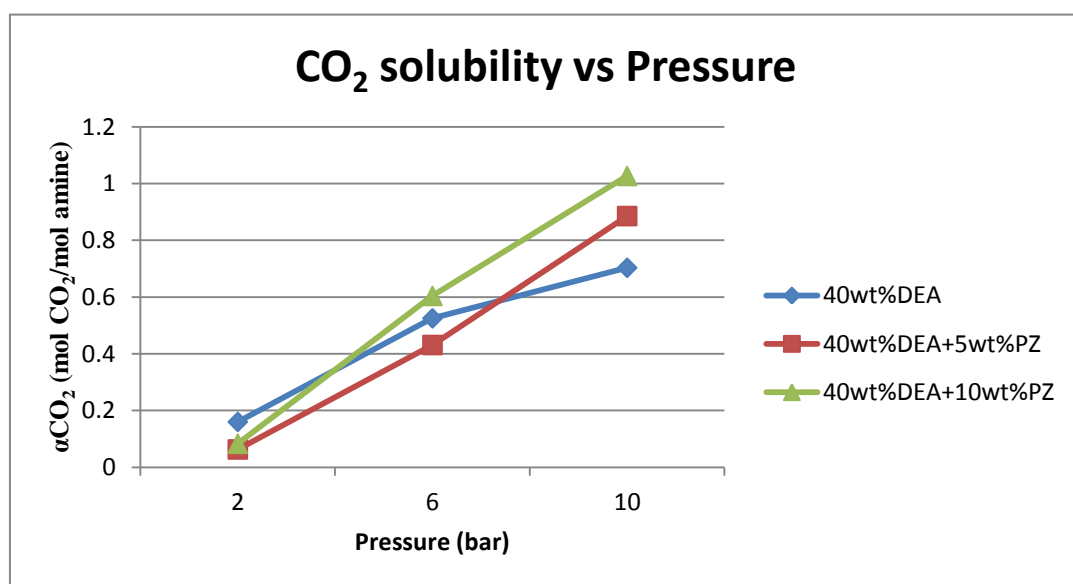


Figure 13: CO₂ loading α_{CO_2} with different mole ratios of PZ at $T = 343.14$ K and $p_{CO_2} = 200$ kPa, 600kPa, 1000kPa for total concentration of amine blend 4M

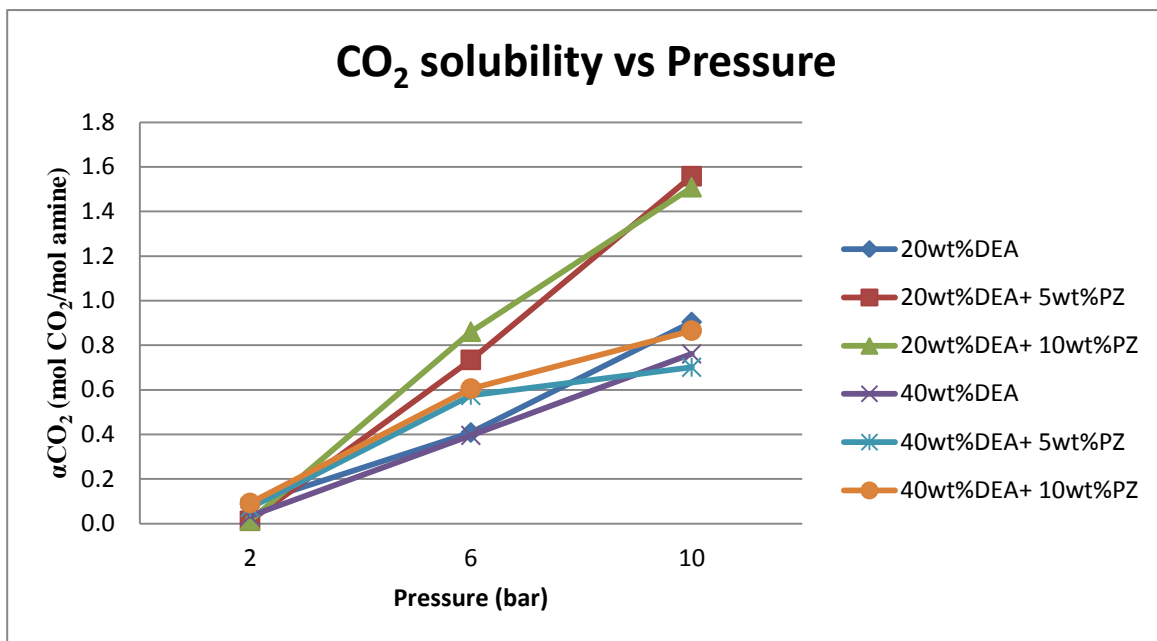


Figure 14: Effect of CO₂ Partial Pressure on CO₂ loading

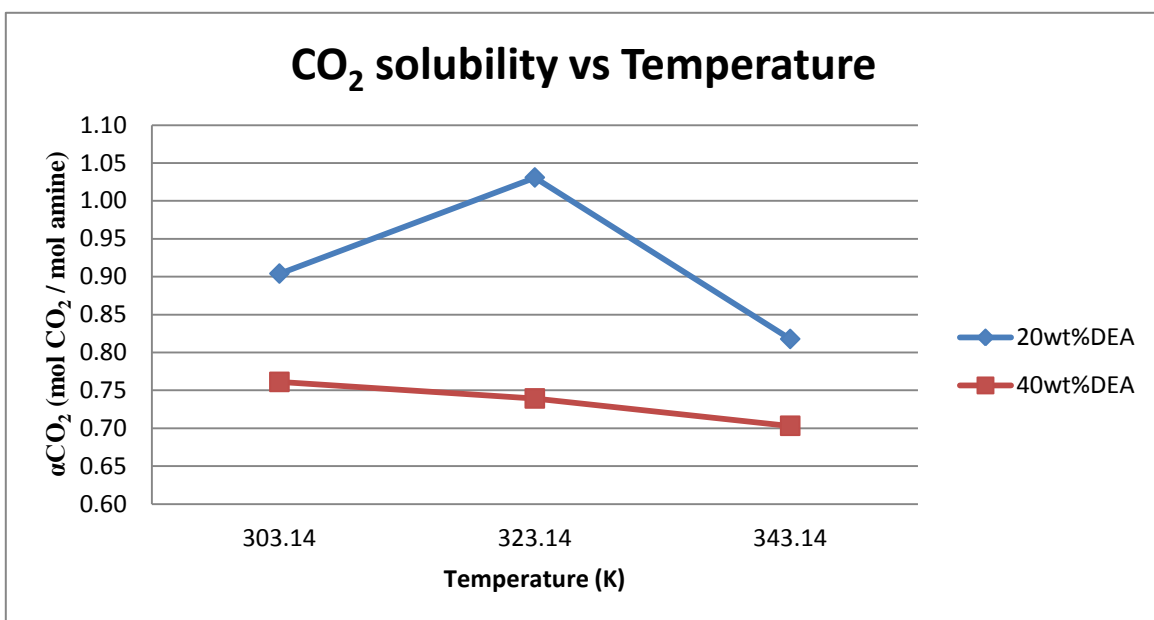


Figure 15: Effect of Temperature on CO₂ loading

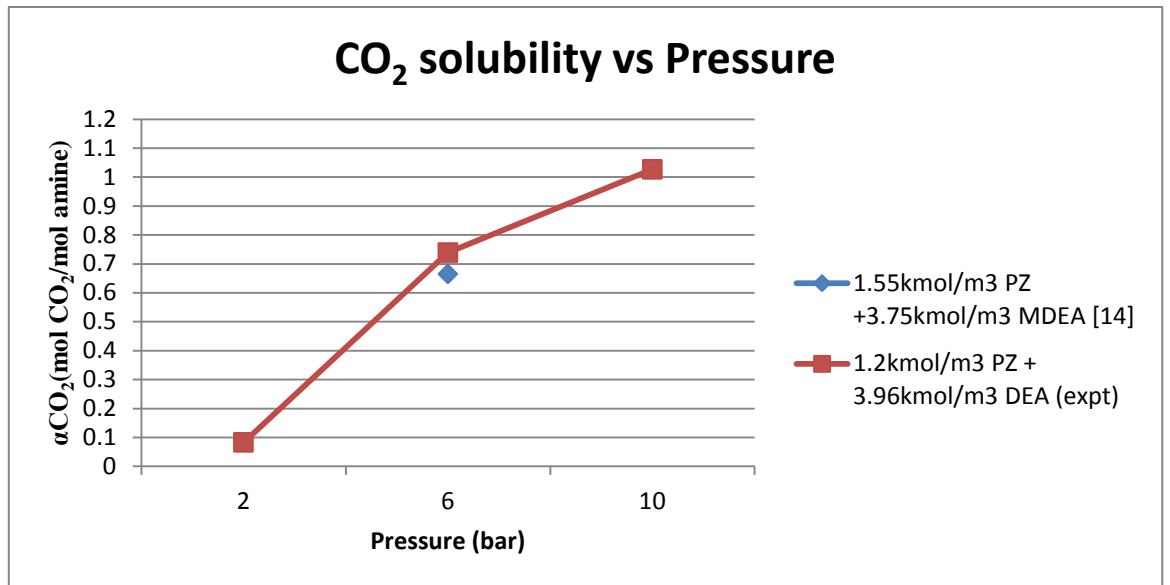


Figure 16: Comparison of CO₂ loading of present study with literature data with different type of blend amine at 343.14K

4.1.2 Refractive Index (n_D) Test Result

Table 7: Result for Refractive Index

Temperature (°C)	20wt% DEA	40wt% DEA	20wt% DEA + 5wt% PZ	20wt% DEA + 10wt% PZ	40wt% DEA + 5wt% PZ	40wt% DEA + 10wt% PZ
30°C	1.36357	1.39167	1.37239	1.38122	1.39979	1.41002
35°C	1.36292	1.39089	1.37174	1.38045	1.39892	1.40918
40°C	1.36205	1.39001	1.37098	1.38796	1.39813	1.40809
45°C	1.36122	1.38876	1.36999	1.37858	1.39688	1.40682
50°C	1.36037	1.38793	1.36927	1.37783	1.39586	1.40588
55°C	1.35962	1.38711	1.36843	1.37668	1.39503	1.40470
60°C	1.35871	1.38608	1.36771	1.37616	1.39407	1.40370
65°C	1.35808	1.38520	1.36672	1.37503	1.39321	1.40286
70°C	1.35693	1.38427	1.36577	1.37423	1.39238	1.40143

4.1.3 Density Measurement ($\rho/\text{g}\cdot\text{cm}^{-3}$) Result

Table 8: Result for Density measurement

Temperature (°C)	20wt% DEA	40wt% DEA	20wt% DEA + 5wt% PZ	20wt% DEA + 10wt% PZ	40wt% DEA + 5wt% PZ	40wt% DEA + 10wt% PZ
25°C	1.0222	1.0461	1.0258	1.0302	1.0501	1.0541
30°C	1.0212	1.0449	1.0252	1.0272	1.0494	1.0536
40°C	1.0170	1.0404	1.0218	1.0264	1.0452	1.0491
50°C	1.0135	1.0378	1.0174	1.0224	1.0402	1.0404
70°C	1.0042	1.0247	1.0058	1.0089	1.0290	1.0268

4.1.4 Viscosity Measurement ($\eta/\text{mPa}\cdot\text{s}$) Result

Table 9: Result for Viscosity Measurement

Temperature (°C)	20wt% DEA	40wt% DEA	20wt% DEA + 5wt% PZ	20wt% DEA + 10wt% PZ	40wt% DEA + 5wt% PZ	40wt% DEA + 10wt% PZ
35°C	1.27	3.26	1.56	2.33	5.02	7.14
50°C	0.93	2.01	1.14	1.57	4.12	6.10
70°C	0.54	1.17	0.85	0.91	2.55	4.95

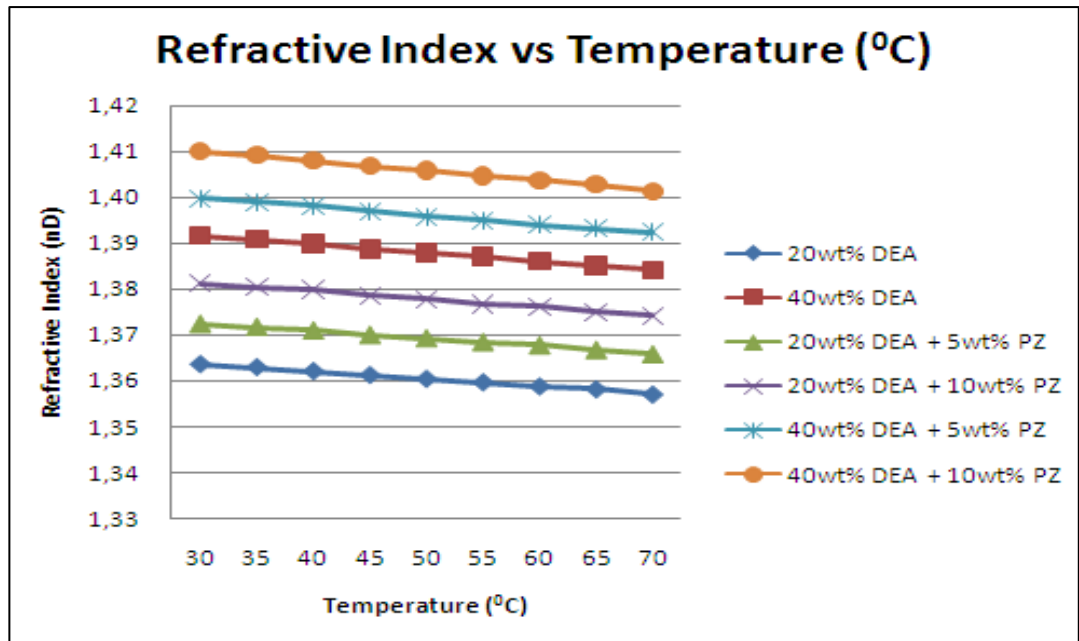


Figure 17: Result for Refractive Index

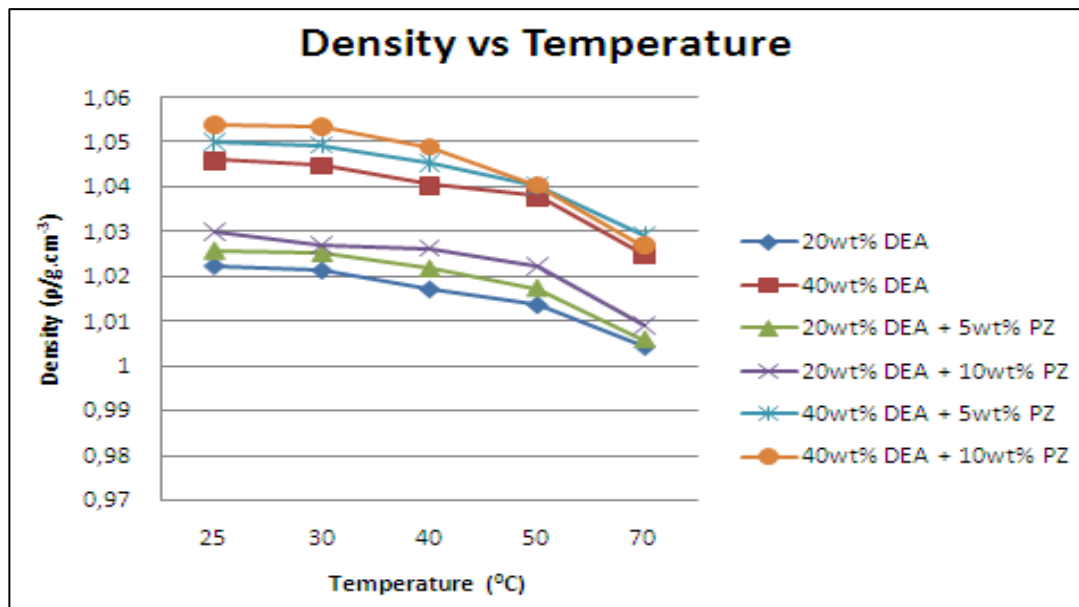


Figure 18: Result for Density measurement

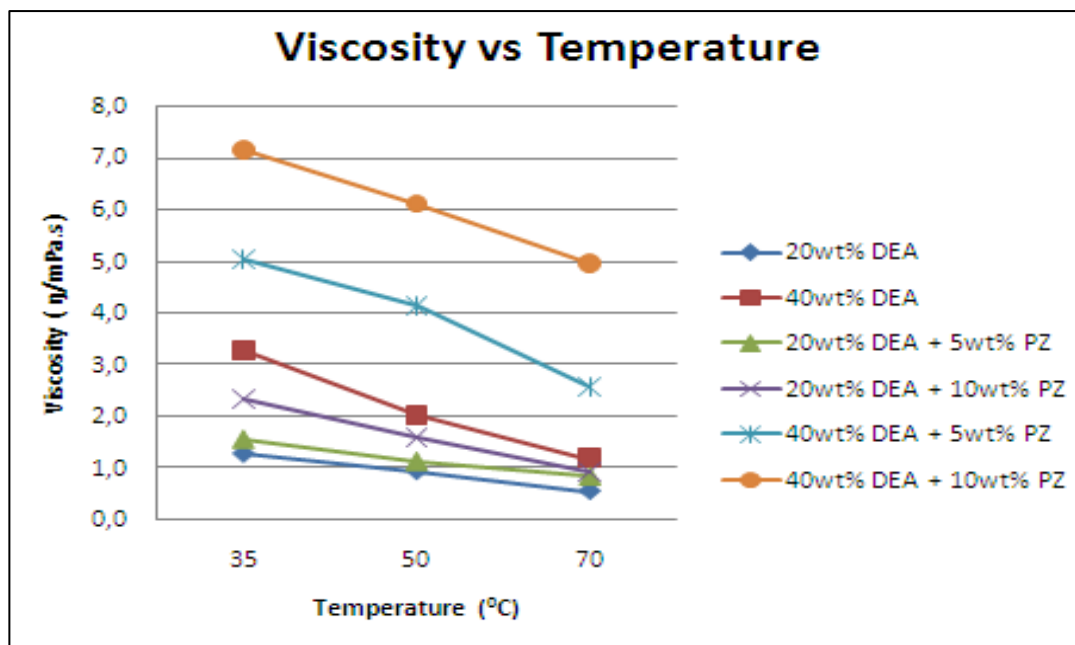


Figure 19: Result for Viscosity Measurement

4.2 DISCUSSION

The solubility of CO₂ in an aqueous blend of DEA and PZ was measured at a concentration of piperazine in total amines between (0.6 and 1.2) at temperature 303.14 K and 200-1000 kPa CO₂ partial pressure as shown in Figure 8. To study the effect of total amine concentration, amine concentration was varied by using 20wt% and 40wt% of amine in the mixture, refer figure 8 and 9. The effect of partial pressure of carbon dioxide P_{CO2} was studied by varying P_{CO2} between (200 and 1500) kPa and can be seen in the figure 13. Figure 15 shows the effect of temperature where temperature was between (303.14 and 343.14) K. The experimental results are listed in Table 4, 5 and 6.

With increasing molar ratio of piperazine in total amine blend, the CO₂ solubility increases at a particular total concentration of amine blend. From Figure 13 solubility of CO₂ increases as the partial pressure of CO₂ in the inlet gas stream is increased at a particular temperature. The effect

of partial pressure of CO₂ in the inlet gas stream is almost the same at all molar ratios of piperazine in total amine blend. For the temperature, from figure 14 the CO₂ solubility decreases at a particular total amine concentration as the temperature increase.

The absorption rate of CO₂ at 30 and 70°C in aqueous DEA with 0.6 to 1.2 M PZ is 1-2 times greater than that in DEA alone. At 40 and 60°C, the CO₂ loading is greater than 0.4 to 0.5 mol CO₂/ mol amine, the equilibrium partial pressure of CO₂ in aqueous DEA with 0.6 to 1.2 M PZ is 1 to 3 times smaller than with DEA alone. At loading less than 0.2 to 0.3, there is no significant effect of PZ on the equilibrium partial pressure of CO₂.

In literature, a lot of amine blends had been worked out for measuring CO₂ loading. Among all of previous work, some of amine blends are compared with the experimental conditions such as partial pressure of CO₂ in inlet gas stream, total concentration of amine blend, and mole fraction of piperazine in amine solution. For comparison purpose, blends consisting MDEA and PZ as one of the component had been used. The CO₂ loading comparisons in experimental data of present study with the other blends are taken at between 3.5 and 4M with the concentration of PZ between 1-1.6 M. From figure 15, it is seen that CO₂ loading is highest for DEA-PZ for present study with experiment condition of 343.14k and 600 kPa.

CHAPTER 5: CONCLUSION AND RECOMMENDATION

5.1 CONCLUSION

In this work, the solubility of CO₂ has been determined in aqueous solutions of (DEA + PZ) for molar ratio of PZ from 0.6 to 1.2M in total amines, temperature range between (303.14 and 343.14) K and partial pressure of CO₂ from (200 to 1000) kPa. The solubility of CO₂ decrease with an increases in temperature and increase with an increase in partial pressure of CO₂ at the given temperature and at a given total amine concentration studied.

Density, viscosity and refractive Index values for aqueous (DEA+PZ) solutions have been measured over a wide temperature range and also correlated. A decrease in all measured physical properties was observed with an increase in temperature.

5.2 RECOMMENDATION

- 1) To compare the solubility of CO₂ experiment result with solubility model values.
- 2) To study the feasibility of having bend DEA/PZ as the removal agent of CO₂ in the gas processing plant.

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APPENDICES

303K/30oC		z= 0,9895								
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading
2,0	20DEA	2,0800	2,0600	1,2900	0,0200	1,0212	0,0024	0,0023	0,0001	0,0122
	40DEA	2,0900	2,0600	1,0200	0,0300	1,0449	0,0037	0,0018	0,0018	0,0924
	20DEA+5PZ	2,0600	2,0400	1,2600	0,0200	1,0252	0,0024	0,0023	0,0002	0,0136
	20DEA+10PZ	2,0400	2,0100	1,2800	0,0300	1,0272	0,0037	0,0023	0,0014	0,0868
	40DEA+5PZ	2,0100	1,9800	1,1300	0,0300	1,0494	0,0037	0,0020	0,0016	0,0714
	40DEA+10PZ	2,2000	2,1800	0,8800	0,0200	1,0536	0,0024	0,0016	0,0009	0,0331

303K/30oC		z= 0,9871								
P(bar)	M	P1	P2	P3	ΔP	density	n CO2(X)	ng CO2(Y)	mol CO2 absorb(Z)	CO2 loading
6,0	20DEA	5,4800	5,3900	2,1600	0,0900	1,0212	0,0110	0,0039	0,0071	0,7342
	40DEA	6,2800	6,1200	4,2200	0,1600	1,0449	0,0196	0,0076	0,0120	0,6055
	20DEA+5PZ	6,1300	6,0000	2,7800	0,1300	1,0252	0,0159	0,0050	0,0109	0,8604
	20DEA+10PZ	6,1800	6,0700	3,9200	0,1100	1,0272	0,0135	0,0071	0,0064	0,4083
	40DEA+5PZ	6,0800	5,9500	1,5600	0,1300	1,0494	0,0159	0,0028	0,0131	0,5744
	40DEA+10PZ	5,9600	5,8400	2,4700	0,1200	1,0536	0,0147	0,0045	0,0102	0,3955

303K/30oC											z= 0,9482
P(bar)	M	P1	P2	P3	ΔP	density	n CO2(X)	ng CO2(Y)	mol CO2 absorb(Z)	CO2 loading	
10,0	20DEA	10,0600	9,8400	6,8800	0,2200	1,0212	0,0281	0,0130	0,0151	1,5581	
	40DEA	10,2800	10,0300	7,8500	0,2500	1,0449	0,0319	0,0148	0,0171	0,8654	
	20DEA+5PZ	10,0600	9,8300	5,4300	0,2300	1,0252	0,0294	0,0102	0,0191	1,5087	
	20DEA+10PZ	9,8600	9,6300	8,0700	0,2300	1,0272	0,0294	0,0152	0,0142	0,9040	
	40DEA+5PZ	10,2500	10,0100	7,7700	0,2400	1,0494	0,0306	0,0146	0,0160	0,7008	
	40DEA+10PZ	10,0200	9,7800	5,8000	0,2400	1,0536	0,0306	0,0109	0,0197	0,7610	

323K/50oC											z= 0,9924
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading	
2	20DEA	2,3300	2,3000	1,4400	0,0300	1,0135	0,0037	0,0024	0,0012	0,1265	
	40DEA	2,3200	2,2800	1,2200	0,0400	1,0378	0,0049	0,0021	0,0028	0,1424	
	20DEA+5PZ	2,2800	2,2500	1,2700	0,0300	1,0174	0,0037	0,0021	0,0015	0,1195	
	20DEA+10PZ	2,2500	2,2200	1,2600	0,0300	1,0224	0,0037	0,0021	0,0015	0,0978	
	40DEA+5PZ	2,2200	2,1900	1,3400	0,0300	1,0402	0,0037	0,0023	0,0014	0,0612	
	40DEA+10PZ	2,1900	2,1600	1,2000	0,0300	1,0404	0,0037	0,0020	0,0016	0,0631	

323K/50oC											z= 0,9765
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading	
6	20DEA	6,3900	6,2600	4,6300	0,1300	1,0135	0,0161	0,0079	0,0082	0,8416	
	40DEA	6,2600	6,1300	2,7000	0,1300	1,0378	0,0161	0,0046	0,0115	0,5801	
	20DEA+5PZ	6,2400	6,1100	4,9200	0,1300	1,0174	0,0161	0,0084	0,0077	0,6051	
	20DEA+10PZ	6,0600	5,9200	1,9500	0,1400	1,0224	0,0174	0,0033	0,0140	0,8941	
	40DEA+5PZ	5,9800	5,8500	2,4300	0,1300	1,0402	0,0161	0,0042	0,0119	0,5230	
	40DEA+10PZ	6,4000	6,2500	1,8700	0,1500	1,0404	0,0186	0,0032	0,0154	0,5938	

323K/50oC											z=	0,9607
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading		
10	20DEA	10,2700	10,0300	7,7300	0,2400	1,0135	0,0302	0,0135	0,0168	1,7263		
	40DEA	10,0300	9,8000	7,8500	0,2300	1,0378	0,0290	0,0137	0,0153	0,7725		
	20DEA+5PZ	9,8200	9,6000	6,2900	0,2200	1,0174	0,0277	0,0110	0,0168	1,3207		
	20DEA+10PZ	10,4100	10,1700	8,0800	0,2400	1,0224	0,0302	0,0141	0,0162	1,0308		
	40DEA+5PZ	10,1800	9,9500	4,8200	0,2300	1,0402	0,0290	0,0084	0,0206	0,9009		
	40DEA+10PZ	9,9700	9,7300	6,3600	0,2400	1,0404	0,0302	0,0111	0,0192	0,7391		

343K/70oC											z=	0,9936
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading		
2	20DEA	2,2500	2,2200	1,5000	0,0300	1,0135	0,0037	0,0024	0,0013	0,1311		
	40DEA	2,2300	2,2000	1,2700	0,0300	1,0378	0,0037	0,0020	0,0016	0,0828		
	20DEA+5PZ	2,2000	2,1700	1,3200	0,0300	1,0174	0,0037	0,0021	0,0016	0,1229		
	20DEA+10PZ	2,1700	2,1400	1,3300	0,0300	1,0224	0,0037	0,0021	0,0015	0,0985		
	40DEA+5PZ	2,6300	2,6000	1,4000	0,0300	1,0402	0,0037	0,0022	0,0014	0,0627		
	40DEA+10PZ	2,6000	2,5500	1,2300	0,0500	1,0404	0,0061	0,0020	0,0041	0,1597		

343K/70oC											Z=	0,9809
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading		
6	20DEA	6,6900	6,5700	5,4400	0,1200	1,0135	0,0148	0,0088	0,0061	0,6241		
	40DEA	6,5700	6,4300	3,3100	0,1400	1,0378	0,0173	0,0053	0,0120	0,6739		
	20DEA+5PZ	6,4300	6,3000	4,0700	0,1300	1,0174	0,0160	0,0065	0,0095	0,7488		
	20DEA+10PZ	6,3100	6,1700	2,6400	0,1400	1,0224	0,0173	0,0042	0,0130	0,8317		
	40DEA+5PZ	6,6200	6,5000	3,0900	0,1200	1,0402	0,0148	0,0050	0,0098	0,4308		
	40DEA+10PZ	6,5300	6,3900	2,2900	0,1400	1,0404	0,0173	0,0037	0,0136	0,5247		

343K/70oC											Z=	0,9701
P(bar)	M	P1	P2	P3	ΔP	density	n CO2 (X)	ng CO2 (Y)	mol CO2 absorb(Z)	CO2 loading		
10	20DEA	10,8000	10,6200	8,9300	0,1800	1,0135	0,0225	0,0145	0,0079	0,8176		
	40DEA	10,6600	10,3900	8,2200	0,2700	1,0378	0,0337	0,0134	0,0203	1,0267		
	20DEA+5PZ	10,3100	10,0500	6,4300	0,2600	1,0174	0,0325	0,0105	0,0220	1,7334		
	20DEA+10PZ	10,6100	10,3400	6,9900	0,2700	1,0224	0,0337	0,0114	0,0223	1,4248		
	40DEA+5PZ	10,3000	10,0500	6,7500	0,2500	1,0402	0,0312	0,0110	0,0202	0,8853		
	40DEA+10PZ	9,8300	9,6100	5,6800	0,2200	1,0404	0,0275	0,0092	0,0182	0,7031		

Calculation of CO₂ loading:-

n_{CO2} transferred to the reactor from the gas container:-

$$\begin{aligned}n_{\text{CO}_2} &= (V_T/R T_a) (P_1/Z_1 - P_2/Z_2) \\ &= [(2.08-2.06)/0.9895](0.083145 \text{ L bar/mol K} \times 298\text{K}) \\ &= 0.0024 \text{ mol}\end{aligned}$$

Where;

V_T is the volume of the container,

Z₁ and Z₂ are the compressibility factors corresponding to the pressure and temperature

P₁ initial pressure before transferring the CO₂

P₂ final Pressure in the gas container after transferring the CO₂ and

T_a is the ambient temperature.

n_{CO2} remaining in the gas phase :-

$$\begin{aligned}n_{\text{g CO}_2} &= (V_{\text{g}} P_{\text{CO}_2} / z_{\text{CO}_2} R T) \\ &= (0.045\text{L} * 1.29\text{bar}) / (0.9895 \times 0.083145 \text{ L bar/mol K} \times 303.14\text{K}) \\ &= 0.0023 \text{ mol}\end{aligned}$$

Moles of C_{O2} in the liquid:-

$$n^1_{\text{CO}_2} = n_{\text{CO}_2} - n_{\text{gCO}_2}$$

$$= 0.0024\text{mol} - 0.0023\text{mol}$$

$$= 0.0001\text{mol}$$

CO₂ loading in liquid phase:-

$$L_{\text{CO}_2} = n_{\text{CO}_2} / n_{\text{AM}}$$

$$= 0.0001\text{mol} / 0.009712$$

$$= \mathbf{0.0122}$$

Where;

n_{AM} is the moles of DEA in the liquid phase