Prediction of Carbon Dioxide solubility in aqueous Methyldiethanolamine (MDEA) solution – A Kent-Eisenberg approach

by

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Dissertation submitted in partial fulfilment of

the requirements for the

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CERTIFICATION OF APPROVAL

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Approved by,

(AP Dr Khashayar Nasrifar)

UNIVERSITI TEKNOLOGI PETRONAS , TRONOH, PERAK

MAY 2013

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

MUHAMMAD AMIRRUL ZAMANI BIN SUHAIMI

ABSTRACT

In this project, the main objective is to develop a model based on the Kent-Eisenberg model to be used with MATLAB software. In this process, the acid component, which is CO_2 gas will be reacted with the alkanolamine solution, aqueous MDEA.

The model is used to predict the loading of CO_2 in aqueous solutions of MDEA under certain sets of parameters such as various temperature (40^0C – 120^0C) and CO_2 partial pressure (0.001 – 1000 kPa). Prediction was also made on the loading in solutions of MDEA based on 35 wt% and also 50 wt%. Prediction also were tested with different sets of MDEA concentration. Besides that, the prediction was compared with the results from the earlier literatures.

In the nutshell, it was found that the model was able to give a relatively good CO_2 loading amount, over wide area of operating conditions as specified with better accuracy than the studied model, Xu et al (1998).

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CHAPTER 1

INTRODUCTION

1.1 Background Study

Carbon Dioxide (CO_2), hydrogen sulphide (H_2S) are categorized as acid gases in the hydrocarbon processing industries. This gases are often present as by-products in industrial gas stream. They are unwanted by-product and often removed for several reasons:

- Improve plant operation and economy
  As this gases appear in large amount, in increases the heat duty, and decreases the plant production capacity
- Reduce equipment operation
  Reaction acid gases with water will lead to severe corrosion of the equipment
- Health, Safety and Environment Issue
  Acid gases are toxic in nature therefore small amount of it may cause harm to humans. CO_2 is an important cause of greenhouse effect

Therefore, the process of removing this gases are called gas sweetening. Normally, a gas sweetening process is chosen depending on the specification on the regulated law available. The components of the gases are shown in table 1.

Table 1: Typical Gas Specification (Wagner et al, 2006)

	CO_2	H_2S
Natural gas	2-3% (v/v)	Less than 4 ppm
LNG	Less than 50 ppm	Less than 4 ppm
Syngas (Oxo)	10 to 100 ppmv	Less than 1 ppm
Syngas (ammonia)	Less than 500 ppmv	-
Refinery	N/A	4 to 150 ppm
Tail Gas	N/A	Less than 250 ppm
Flue Gas	85 – 95% removal	•

The sweetening process is crucial for further refining and manufacturing process. A general amine gas treatment facility includes an absorber unit and also regenerator unit and other equipment. As this project only focuses on the removal of CO2 gases from the streams, this paper will not be discussing further on the configuration of the facility.

Nowadays, aqueous alkanolamine solution is widely used in the CO2 capture and removal from acid gas streams. In industry, MDEA solutions are the most used alkanolamine absorbents as it is cheap, having higher loading capacity, used less energy to regenerate and also have high resistance to thermal and chemical degradation.

It is found that, vapor-liquid equilibrium (VLE) is the most important data for the prediction of the loading amount of CO2 in alkanolamine solution. In earlier works, numerous VLE studies have been conducted experimentally and theoretically, and numerous models was created to predict the VLE relationship for the alkanolamine solutions.

The first mathematical model was proposed by Kent and Eisenberg (1976). This model was used because of its simplicity in computation. In this model, it is assumed that all activity and fugacity coefficient is in ideal state. This assumption forces the model and experimental results to be fitted into two equilibrium constants (K1 and K2) as additional parameters. Although it is simple, the limitation for this model is limited extrapolation applicability outside of its validity range.

The modification on the original model was done in this paper. The free gas concentration in the solution and amine concentration was added into the original model. This additional variables was added in order to produce better prediction on the total CO2 loading in the amine solution. Therefore, with this modification, it is hope that this model is able to predict the CO2 solubility in amine solution at higher pressure and also temperature. Later in this work, the prediction was compared with data from Jou et al (1982) and Xu et al (1998).

1.2 Problem Statement

The prediction of CO2 solubility in aqueous MDEA solution at higher operating pressure (0.001 kPa – 1000 kPa) and temperature (40^0C – 120^0C) is still not developed yet. Therefore, this paper's model is used to predict the solubility of CO2 in aqueous MDEA solution in high pressure-temperature region and the results is compared with Jou et al (1982) and Xu et al (1998) to find the performance of this model.

1.3 Objective of the Study

- To develop a model that predict the solubility of CO_2 over aqueous methyldiethanolamine (MDEA) solution with respect of Kent-Eisenberg model
- Examine the developed model performance under high pressure, high temperature and also high concentration region by comparing to the experimental data of Jou et al (1982) and Xu et al (1998) based on the error analysis

1.4 Scope of Study

In this study, the main subjects under investigation are:

- The solubility of CO_2 over MDEA solution
- Absorption of CO_2 shown by Kent-Eisenberg model that describes the partial pressure of CO_2 in narrowed conditions

CHAPTER 2

LITERATURE REVIEW

2.1 Fight against Carbon Dioxide

The fight against global climate change always will be the difficult ones for human community. As the population increases, the demand for energy increases. Thus, increases the CO_2 production as it is largely produced by energy generation industries. In addition to that, other industries such as steel production, chemical production and etc. also leads to the influx of CO_2 in atmosphere. For that, numerous intensive researches and studies were made on CO_2 capture and sequestration.

CO_2 is generally known as a molecule consist of one carbon atom bonded to two oxygen atoms. At standard atmospheric condition, it is identified as a colourless, odourless gas that also plays an important role in Earth's atmosphere warming system and it also plays a major role in carbon cycle. The generation of CO_2 can be also in natural state and also anthropogenic. Naturally, oceans, forests, and other biota acts as earth's carbon sinks just to balance out the amount of CO_2 in the atmosphere. The removal process of CO_2 is not only because to reduce the amount of greenhouse gases, but also to fulfil the needs of technical and economic concerns of industries. When present in natural gas, Carbon dioxide will reduce the heating value of the gas. In addition, it also have tendency to cause corrosion inside a pipeline, equipment and also catalyst as in ammonia synthesis process (G. Astarita et al. 1983). In the past, CO_2 removal from the gas streams is viewed as an alternative method for enhanced oil recovery (EOR) operations. Besides that, the recovered CO_2 is used in welding industry, food and beverage industry, and also soda ash industry. Although there are some demands over the produced $CO_{2,}$ the production keep increasing and polluted the environment. As the time progresses, people are becoming aware on the environmental importance, therefore the CO_2 capture and sequestration were born.

Currently, there are many technologies exist for CO_2 capture and sequestration process. Technologies such as physical adsorption, chemical absorption, gas permeation, and also physical absorption (A.L. Kohl, 1997). In this paper, the attention of the technology used for capturing CO_2 will be directed to the absorption process as it is more economical. Physical absorption is the most common practice nowadays. It have no limitation on the absorptivity capacity and also it is more economical. The solubility of CO2 is governed by the VLE of the mixture, which are affected by pressure and temperature. It is found that at higher pressure, it is more efficient to use physical absorption process compared to chemical absorption. Therefore, this paper will be focusing more on this.

2.2 Usage of Alkanolamines

Latest practice in removing of CO_2 in today's industries is by using aqueous solution of alkanolamine as the chemical absorbents. This technique has been proven to be efficient and reliable, which applicable in every chemical process which produces CO_2.

Alkanolamine can be categorized into primary, secondary, and tertiary amine depending on the number of attached alkyl group to its structures. Studies shows primary and secondary amine have low CO_2 loadings (mol of CO_2 per mol of amine). However, they have high rate of absorption. In contrast to the tertiary amine which shows the opposite behaviour from both primary and secondary amine. In the end, the choice of a particular amine will depend not only on the absorption rate and maximum loading that can be achieved, but also on other factors such as regeneration energy, corrosion tendency and the cost of the solvent.

Aqueous monoethanolamine (MEA) and aqueous methyldiethanolamine (MDEA) are the most used amine solutions as they are relatively low in cost, very stable, and have higher capacity of loadings. In between of these two, MDEA is preferred because it have higher loading capacity, less regeneration energy, and high resistance to thermal and chemical degradation.

MDEA can be found in clear, colourless, or sometimes in pale yellow liquid with an ammonia scent. Naturally, it is miscible in water, alcohol and also benzene. It is categorized as tertiary amine.

2.3 Prediction of Carbon Dioxide Solubilities

The first acid gas – alkanolamine systems available does not consider activity coefficient. In Van Krevelen et al (1949) work, they proposed an “apparent” equilibrium constant in their VLE model, which used concentration instead of activities. This equilibrium constant is further supported with experimental data with a function of ionic strength. This method is further developed by Danckwerts et al (1967).

The Dackwerts et al (1967) approach to the solubility of acid gases in aqueous solution of MEA and DEA is later adapted by Kent and Eisenberg (1976). This model proposed a set of non-linear equations which has to be solve simultaneously. In this model, the non-idealities is lumped together, in chemical equilibrium constants and used in the model. Besides that, the following component balances are also need to be solved simultaneously.

Amine balance:

$[RR'NH]_t = [RR'NH]_e + [RN'NCOO-]_e$ Equation 1

CO_2 balance:

$a[RR'NH]_t = [HCO_3-]_E + [RR'NCOO-]_e + [CO_3^{2-}]_E + \frac{Pco2}{Hco2}$ Equation 2

Electron balance:

$[RR'NH_2^+]_t = [HCO_3^-]_e + [RR'NCOO^-]_E + 2[CO_3^{2-}]_e$ Equation 3

The parameter α is the acid gas loading, which in this thesis is CO_2 loading. The concentration of molecular CO_2 in the liquid phase is estimated with Henry's law.

$P_{CO2} = H_{CO2}[CO_2]$ Equation 4

Based on W. Hu and A. Chakma (1990) studies, the equilibrium constant at infinite dilution, K_1 is a function of temperature, a factor F_1 was introduced which takes the effects of CO_2 partial pressure and the amine concentration into account. For that, reaction (1) and (2) are defined into an apparent equilibrium constant, K'_1 which shows the effect of partial pressure of CO_2 and the amine concentration in the solution. Thus,

$K'_1 = K_1 F_1$ Equation 5

In this paper, F_1 is defined as:

Equation 6

$$F_1 = e(\frac{r_i}{P_{CO2}} + g_i ln P_{CO2} + h_i ln P_{CO2} + \frac{j_i}{[RR'NH]} + k_i \ln[RR'NH] + m_i[RR'NH]$$

The chemical equilibrium data used for comparison are published in open literature, except for the ones consist of amine protonation and carbamate formation reaction. For that, a data from study based on M.Z Haji Sulaiman et al (1998) paper was used. It was proposed that for the protonation of amine, only g_i and k_i are important and for the formation of carbamates, the contribution from g_i and j_i are significant. Based on the idea proposed by the paper, F_i is expressed as:

Protonation of amine

$F_i = g_i \ln P_{CO2} + k_i \ln [RR'NH]$ Equation 7

Formation of carbamate

$F_i = gi \ln P_{CO2} + \frac{ji}{[RR'NH]}$ Equation 8

Therefore, in this paper, using these equilibrium constants to fit the parameters, the calculated acid gas partial pressure is forced to converged the available experimental VLE data for single gas – single amine experiments.

2.4 Vapour Liquid Equilibrium Model Framework

For this framework, this study follows back the equilibrium reaction of CO_2 – MDEA – H_20 system by Austgen et al. (1991):

Ionization of water $MDEA + H^+ \overset{k1}{\leftrightarrow} MDEAH^+$ (1)

Dissociation of Carbon Dioxide $CO_2 + H_2O \overset{k2}{\leftrightarrow} HCO_3^- + H^+$ (2)

Ionization of water $H_2O \overset{k3}{\leftrightarrow} OH^- + H^+$ (3)

Dissociation of bicarbonate $HCO_3^- \overset{k4}{\leftrightarrow} CO_3^{2-} + H^+$ (4)

Reaction (1) – (4) completely define the CO_2 system which must be taken into consideration when designing the system. Chemical equilibrium (phase and reaction equilibrium) for this system, including phase equilibrium, reaction equilibrium, electro neutrality, and mass balance.

The stoichiometry equilibrium constants for main reaction of CO_2-MDEA-H_2O system can be written as:

$$k_1 = \frac{[H^+][MDEA]}{[MDEA^+]} \qquad (5)$$

$$k_2 = \frac{[H^+][HCO_3^-]}{[CO_2]} \qquad (6)$$

$$\begin{gathered} k_3 = [H^+][OH^-] \\ k_4 = \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} \end{gathered} \qquad (7)$$

Phase equilibrium is represented by Henry's Law:

$$\mathrm{P}_{\mathrm{CO2}} = \mathrm{H}_{\mathrm{CO2}}[\mathrm{CO}_2] \qquad (8)$$

Electro neutrality balance of the ionic reaction is represented by:

$$[MDEAH^+] = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] + [H^+] \qquad (9)$$

The mass balance of electrolyte is aqueous phase is given by following equation:

$$\alpha[MDEA]_t = [CO_2] + [HCO_3^-] + [CO_3^{2-}] \qquad (10)$$

$$\alpha[MDEA]_t = [CO_2] + [HCO_3^-] + \frac{k_4[HCO_3^-]}{[H^+]} \qquad (11)$$

$$\alpha[MDEA]_t = [CO_2] + \frac{k_2[CO_2]}{[H^+]} + \frac{k_2 k_4[CO_2]}{[H^+]^2} \qquad (12)$$

Where C is the concentration of species in kmol.m^{-3}. The VLE calculation is represented by simultaneous solution of the above equation.

2.5 Conclusion

This paper is using the Kent-Eisenberg model to predict the CO_2 solubilities in aqueous MDEA solutions. In this work, the equilibrium constant was expressed as a function of amine concentration, amine loading, acid concentration and temperature. The model was regressed against the published experimental data over the conditions stated, and were validated.

CHAPTER 3

3.1 Methodology and Project Work Plan

The following flowchart shows the general experimental procedures that will be implemented in this project:

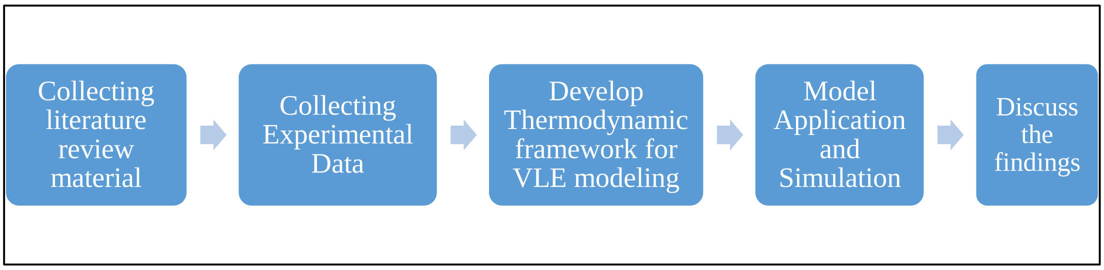

Figure 1: The schematic diagram depicting general approach in this project

3.2 Key Milestone

Several key milestones for this research project must be achieved in order to meet the objective of this project

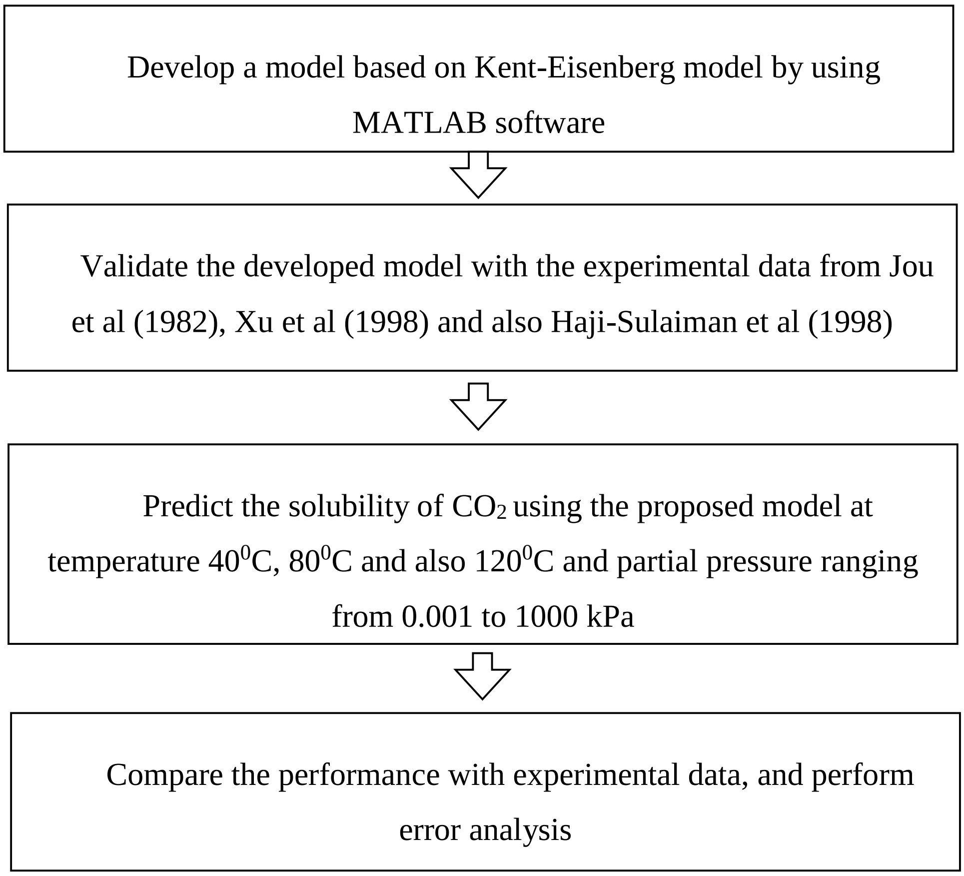

Figure 2: The schematic diagram depicting the key milestone for this project

This project is mainly to develop a mathematical framework that utilizes the Kent-Eisenberg original model to analyse the solubility of CO_2 gas in the MDEA solution. The development of this application has been done using the MATLAB.

Next, the developed model was tested and verify with the experimental data from Haji-Sulaiman et al (1998). This is to test the proposed model in order to ensure that the developed model is working. The parameters tested on the model are pressure ranging from 0.001kPa to 1000kPa, temperature of 40^0C to 120^0C, and also weight percentage of the MDEA.

Next phase was to predict the solubility of CO_2 using the final MATLAB model at temperature 40^0C to 120^0C and partial pressure from about 0.001 to 1000 kPa, with reference to Xu et al. (1998). After the MATLAB coding has been validated and verified for its workability, the parameters and data were fitted into the model. The prediction data was then recorded for the next error analysis phase

After that, the prediction data from the developed model was compared with the experimental data by using error analysis method. The method was done using the following equation:

Error % = $[{}^{\propto p - \propto exp}/_{\propto exp}]$ X 100%

Where

αp = predicted CO_2 loading

αexp = experimental CO_2 loading

In the end, the model is analysed from its error analysis. If the error is lower than the model proposed by Xu et al. (1998) model, it can be concluded that this model is better than the one proposed by Xu et al. (1998).

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Validation of the Model

As the completion of the proposed model, it was tested for the solubility data of CO_2 in aqueous MDEA solution. The parameter involved during this testing are, weight percentage (35wt% and 50wt %), temperature (40^0C, 80^0C, 120^0C) and also pressure (0.001kPa to 1000kPa). Figure 3 shows the data generated from the developed model. α(exp) is the data published by Xu et al (1998) meanwhile α(calc1) were CO_2 loading data generated by Haji-Sulaiman et al (1998) and α(calc2) are CO_2 loading data generated by the model proposed by this paper.

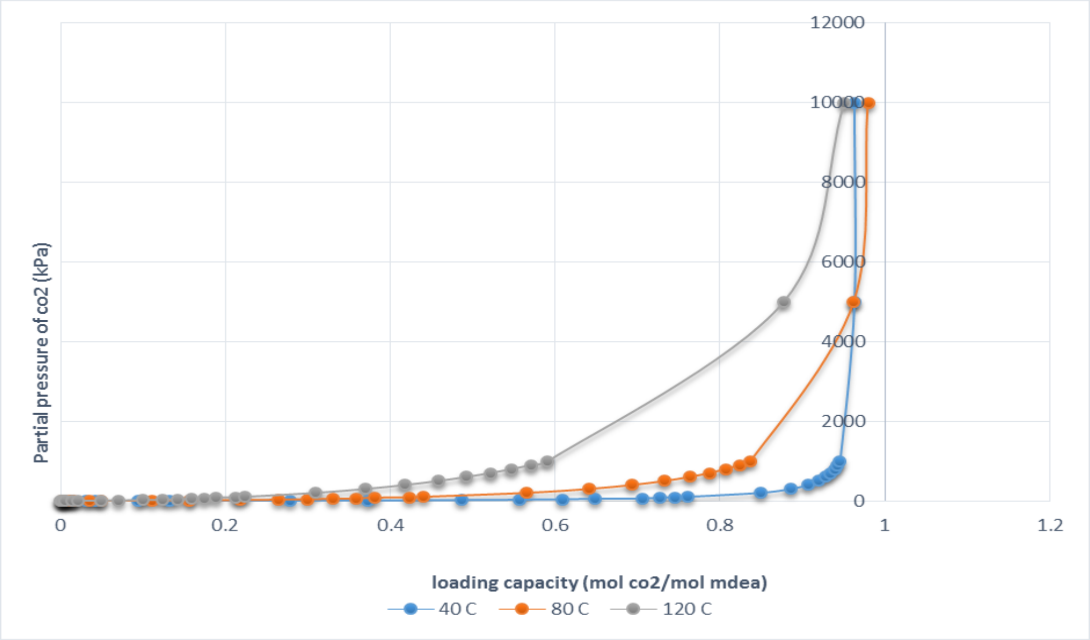

Figure 3: Graph of loading capacity in 35wt% of MDEA against CO_2 partial pressure

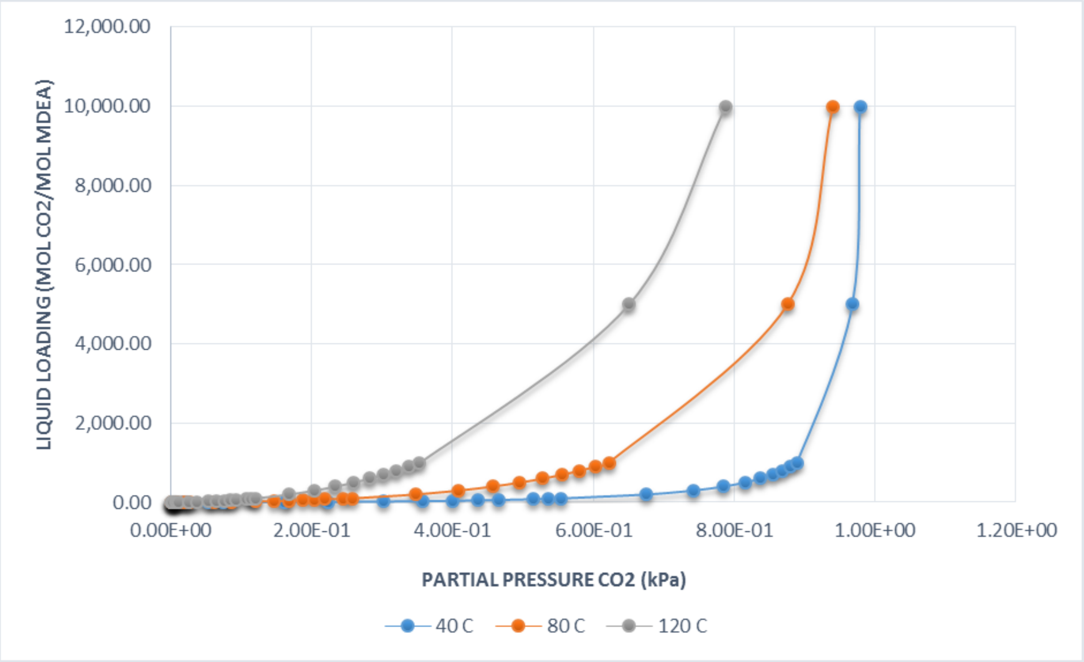

Figure 4: Graph of loading capacity in 50wt% of MDEA against CO_2 partial pressure

For this model to be accepted, it must follow this two condition:

- Range of CO2 loading in MDEA is in range of 0 to 1.0
- The deviation between model data and experimental data must be lower than 30%

From the results produced, the range of CO_2 loading in MDEA is in range of 0 to 1.0 mol, which is the acceptable range of the loading data. The model mathematical derivation also was checked with the derivation as in H. Pahlavanzadeh et al (2011) paper. As observed in α (calc2) data, the average deviation from the experimental data proposed by Xu et al (1998) is 12.3% for 35 wt% and 23% for 50wt% of MDEA solution. The deviation percentage are shown in the figure below:

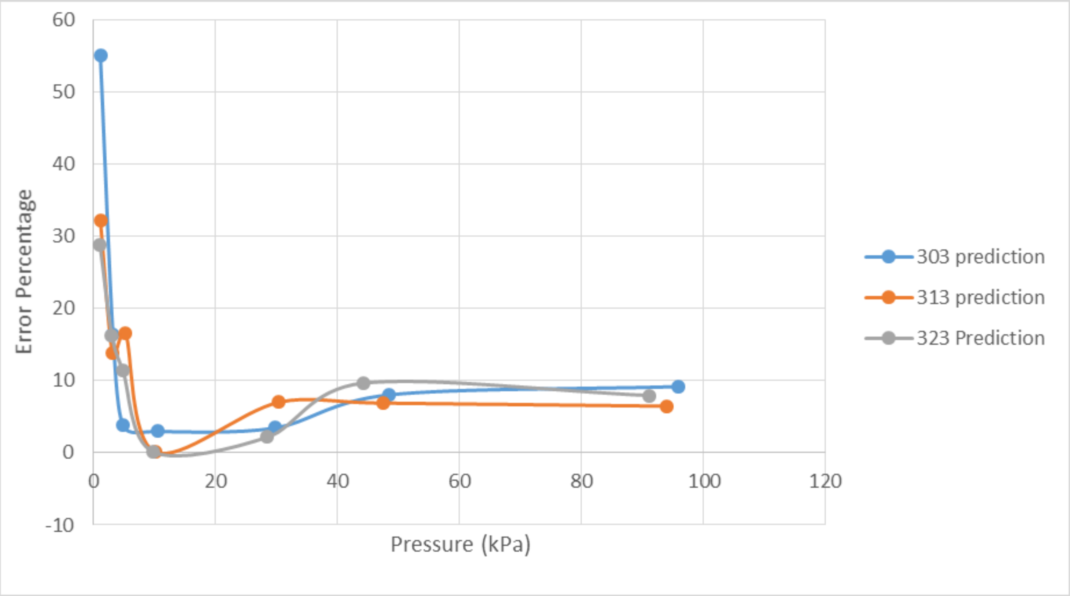

Figure 5: Error percentage of CO2 loading in 35wt% MDEA solution

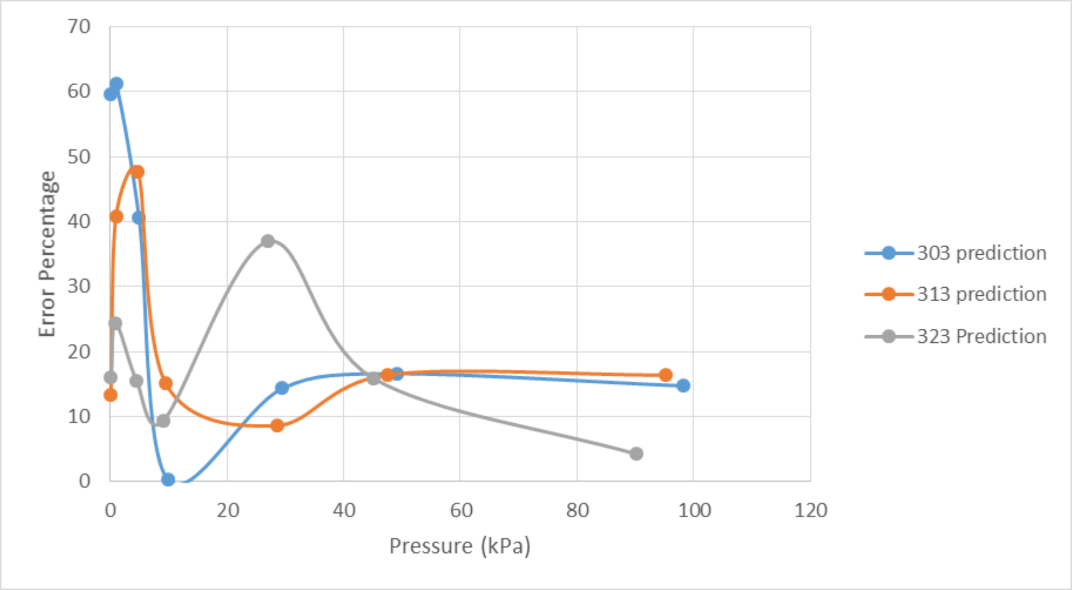

Figure 6: Error percentage of CO2 loading in 50wt% MDEA solution

With the model follows both of the conditions aforementioned, the model proposed by this model is valid and can be used for further data modelling at higher temperature and higher pressure.

4.2 Modelling of CO$_2$ loading at higher pressure, higher temperature and higher molarity

After the model was validated at lower working temperature and pressure, the proposed model was tested with amounts of 3.04M, 3.46M, 4.28M concentration of MDEA solution, 40^{0}C (313K) to 100^{0} C (373K) of temperature, and also 10 – 1000 kPa of CO2 partial pressure. This data were later compared to the data provided by Xu et al (1998). Below shows the graphs generated from the modelling.

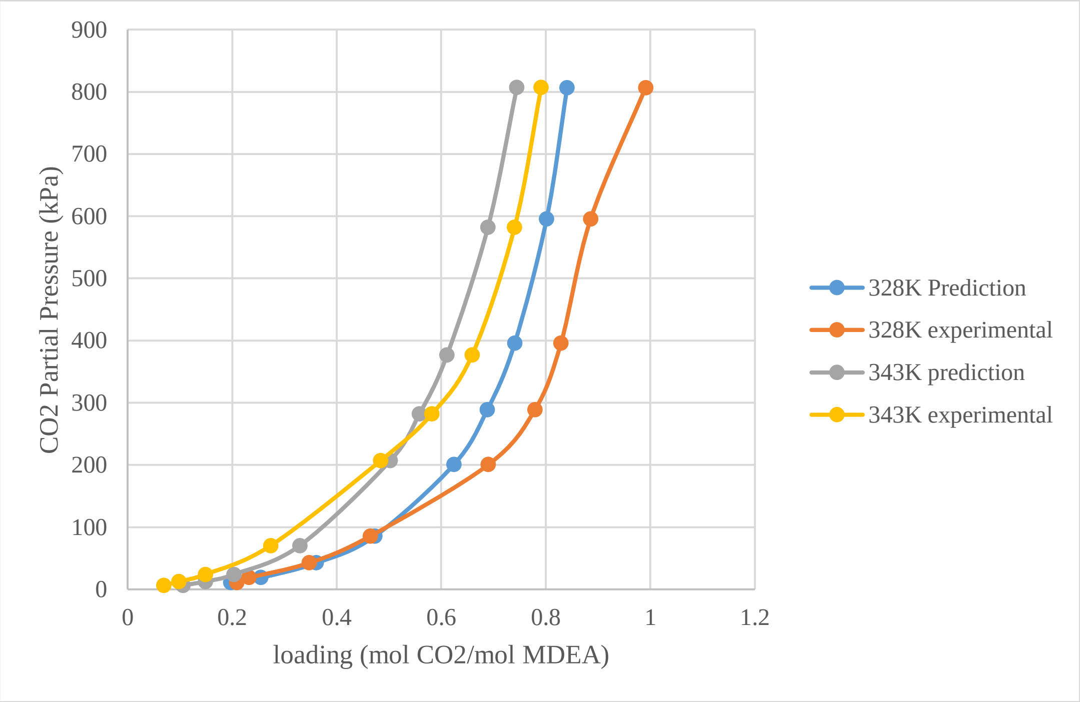

Figure 7: loading of CO$_2$ inside 3.04M of aqueous MDEA solution

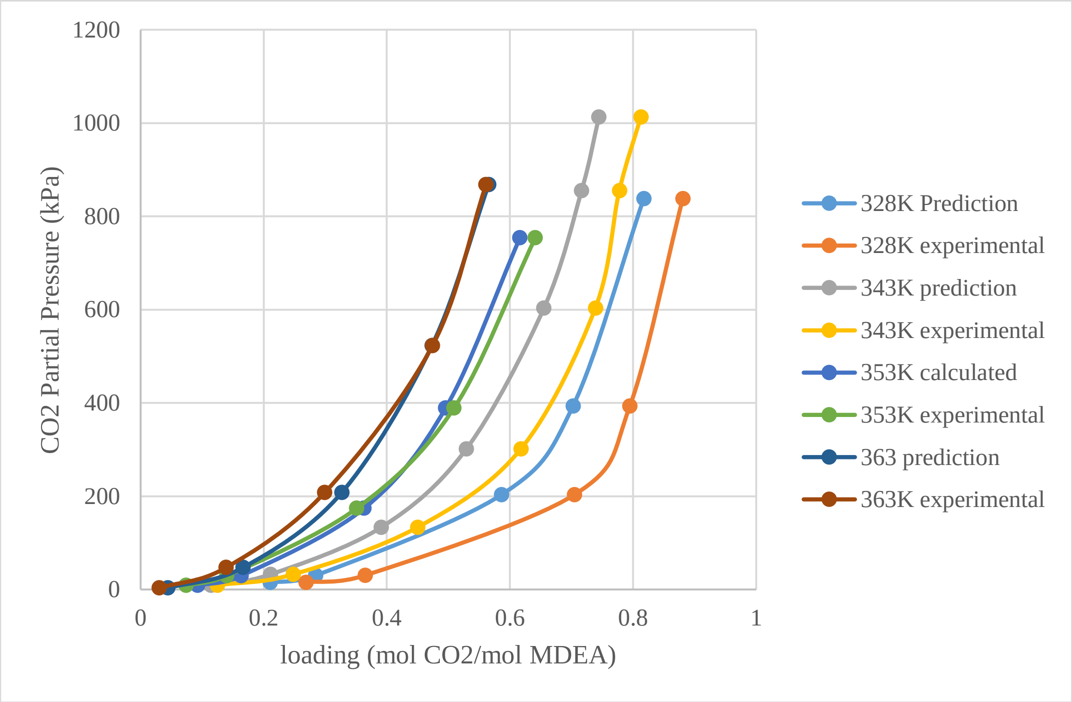

Figure 8: loading of CO_2 inside 3.46M of aqueous MDEA solution

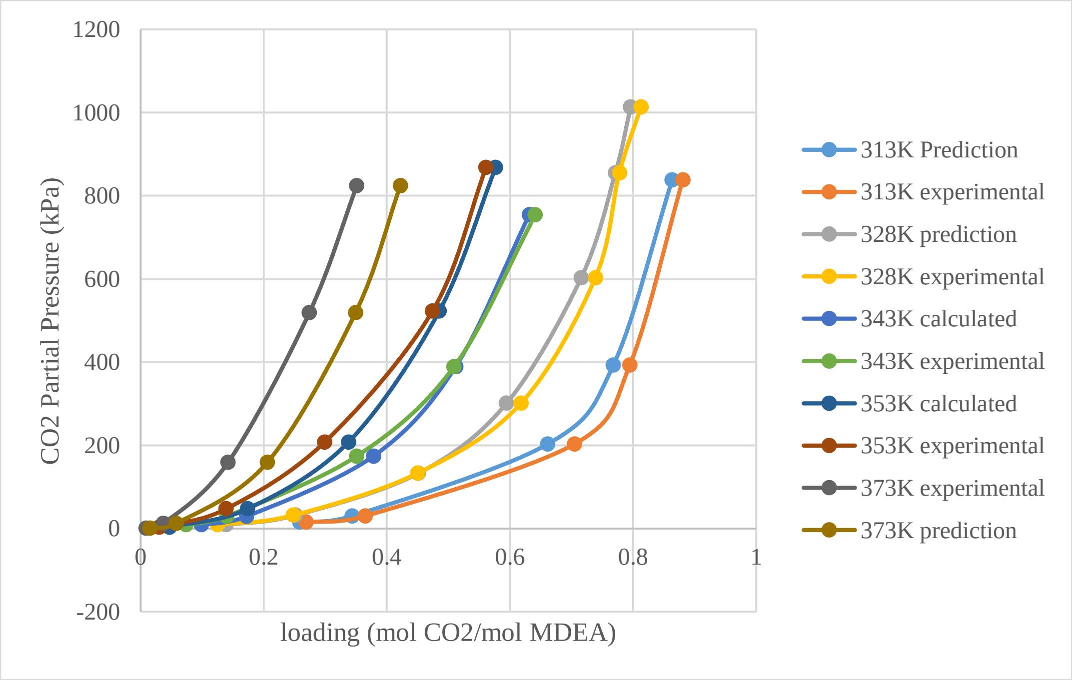

Figure 9: loading of CO_2 inside 4.28M of aqueous MDEA solution

4.3 Deviation analysis of the model

In general, within the range of parameters tested above, the predicted and published data shows good agreement with a maximum deviation of 14.6%. Relatively, high deviations which is 21%, is shown when the data is regressed under low concentration of MDEA used, and high temperature.

It also found that in general, as the CO_2 partial pressure is increased, a higher loading is also achieved. This can be shown on the trends in the above graphs. However, the loading of CO_2 is also affected by the effect of the temperature. From the result produced, it can be concluded that upon increasing the temperature, the loading decreases. Besides that, from the deviation analysis made, it is note that the error percentage increases as the temperature increases. Below are the graphs produced from the error analysis.

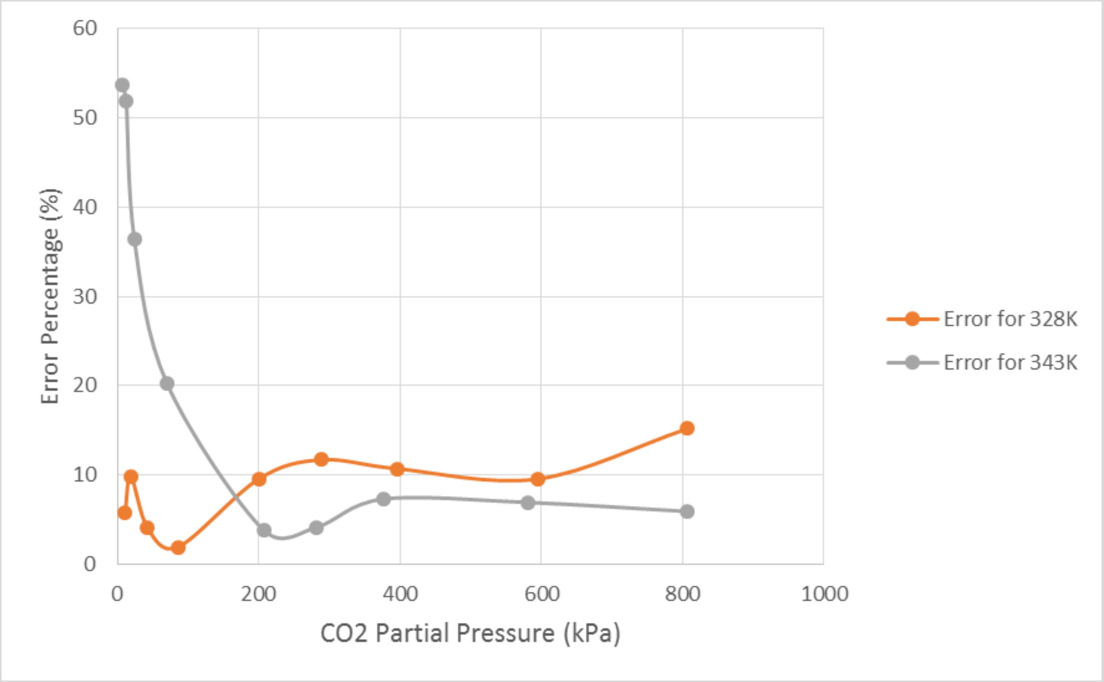

Figure 10: Graph of error analysis of 3.04M aqueous MDEA solution

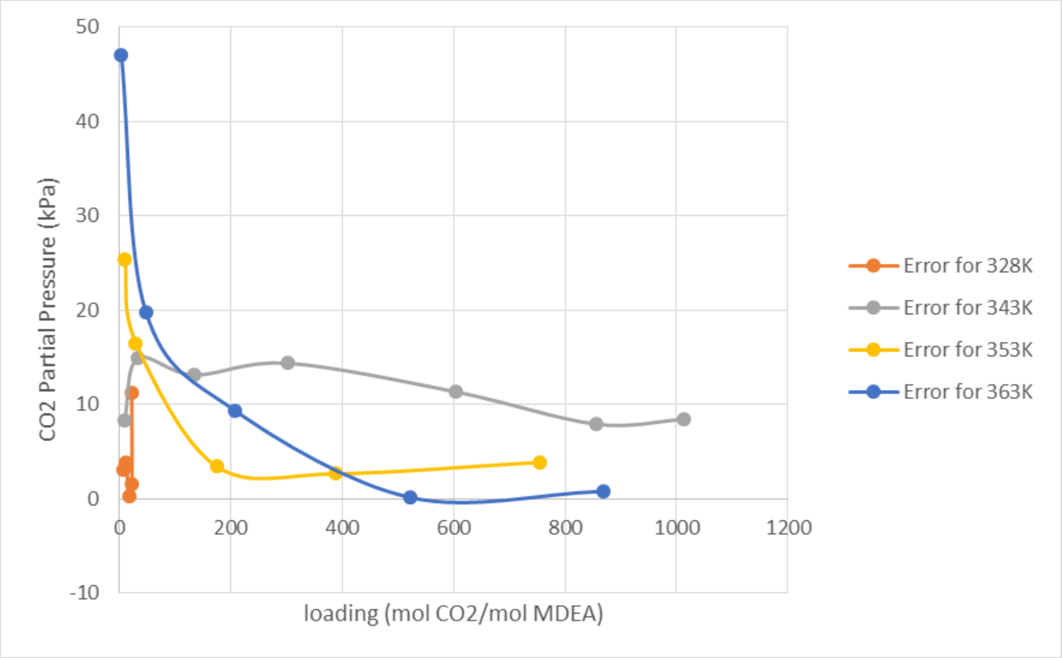

Figure 11: Graph of error analysis of 3.46M aqueous MDEA solution

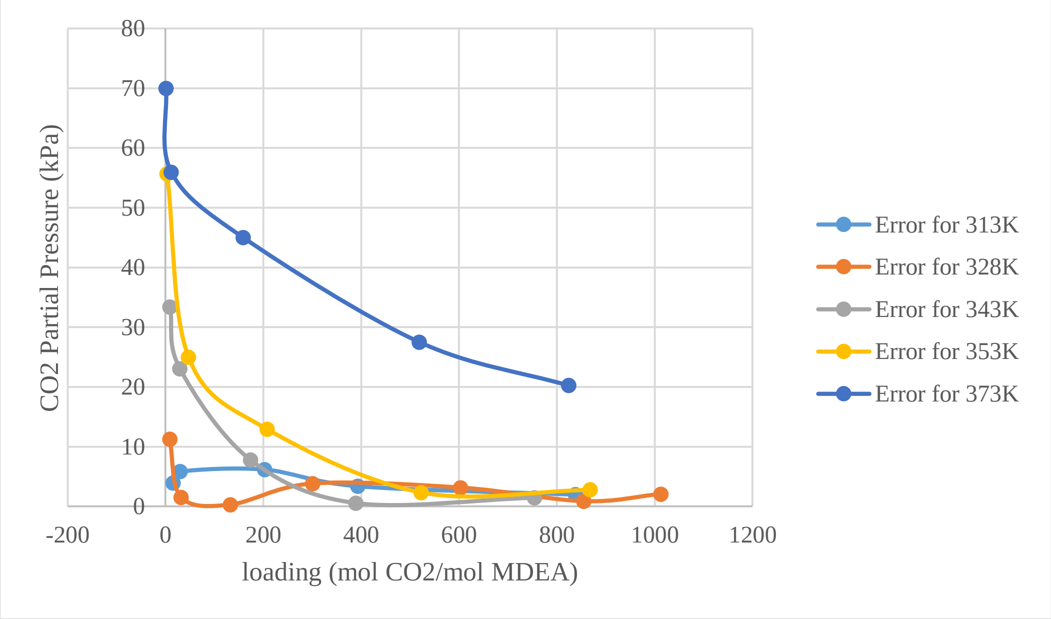

Figure 12: Graph of error analysis of 4.28M aqueous MDEA solution

From the observation and data produced, it is recommended that the model is refitted with more data which conducted at higher CO_2 partial pressure and also higher temperature. This is to give the model an improvement in terms of accuracy of the calculated data.

CHAPTER 5:

CONCLUSION

It is concluded that the model is considered to be giving a good prediction on CO_2 solubility data in aqueous solution of MDEA at higher range of temperature (40^0C – 120^0C), high pressure range (0.001 kPa – 1000 kPa) and also at different concentration of MDEA (3M – 4M) as well.

It is observed that as pressure increases, the loading capacity increases as well with a significant decreases in data deviation. However, due to restriction in data, the prediction can only be made until 1000kPa. For that, it is recommended for future studies on CO_2 solubility at higher partial pressure of CO_2. This is to give a better and improved accuracy in prediction of the model in future studies.

Besides that, it is also observed that at higher temperature used, the percentage of error is increasing as the temperature increases. Again, due to limitation of data, this model can only do prediction from 40^0C until 120^0C. It is also recommended that this model is reassessed in terms of addition of temperature effects inside the factor F_i.

In the nutshell, based on the performance analysis with Xu et al (1998) experimental and predicted data, it is concluded that this better is considered as better since this model only produces an average error of 14.6% compared to the model proposed by Xu et al (1998) which yielded 17.91% of deviation.

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APPENDIX I: Predicted Carbon Dioxide solubilities in 35 wt% of MDEA

Table 2: Predicted Carbon Dioxide solubilities in 35 wt% of MDEA

Mol (M)	2
T(K)	313.5
kPa	alpha (mol CO2/mol MDEA)
0.001	0.0049
0.01	0.014
0.05	0.0303
0.1	0.0426
0.5	0.0939
1	0.1316
5	0.278
10	0.3729
20	0.4859
30	0.5574
40	0.6088
50	0.6482
60	0.7054
80	0.727
90	0.7453
100	0.7612
200	0.8489
300	0.8861
400	0.9065
500	0.9192
600	0.9279
700	0.9341
800	0.9388
900	0.9424
1000	0.9453
5000	0.9627
10000	0.9625

APPENDIX II Predicted Carbon Dioxide solubilities in 50 wt% of MDEA

Table 3: Predicted Carbon Dioxide solubilities in 50 wt% of MDEA

Mol (M)	4
T(K)	313.5
kPa	alpha (mol CO2/mol MDEA)
0.001	2.90E-03
0.01	0.0081
0.05	0.0173
0.1	0.0241
0.5	0.0531
1	0.0746
5	0.1618
10	0.2226
20	0.3018
30	0.3571
40	0.4002
50	0.4357
60	0.4658
80	0.5151
90	0.5356
100	0.5542
200	0.6757
300	0.742
400	0.7848
500	0.815
600	0.8374
700	0.8548
800	0.8687
900	0.8801
1000	0.8895
5000	0.9682
10000	0.9789

APPENDIX III: Predicted Carbon Dioxide solubilities in higher parameters

Note: The predicted solubilities are tested and validated with data from Xu et al (1998).

1. Mol: 3.04M

Temperature: 55^0C

Table 4: Predicted Carbon Dioxide solubilities at 3.04M in 55^0C

M	T (K)	PCO2e	a expt	a calc	Error %
3.04	328	10.74	0.209	0.1971	5.69378
		18.85	0.232	0.2547	9.784483
		42.57	0.347	0.361	4.034582
		85.57	0.464	0.4728	1.896552
		200.5	0.69	0.624	9.565217
		288.5	0.779	0.688	11.68164
		395.5	0.829	0.7404	10.68758
		595.5	0.886	0.8015	9.537246
		806.5	0.991	0.8407	15.1665

2. Mol: 3.04M

Temperature: 70^0C

Table 5: Predicted Carbon Dioxide solubilities at 3.04M in 70^0C

M	T (K)	PCO2e	a expt	a calc	Error %
	343	6.15	0.069	0.1061	53.76812
		12.33	0.098	0.1489	51.93878
		23.79	0.149	0.2033	36.44295
		70.17	0.274	0.3294	20.21898
		206.8	0.484	0.5024	3.801653
		281.8	0.582	0.558	4.123711
		376.8	0.659	0.611	7.283763
		581.8	0.74	0.689	6.891892
		806.8	0.791	0.7444	5.891277

3. Mol: 3.46M

Temperature: 55^{0}C

Table 6: Predicted Carbon Dioxide solubilities at 3.46M in 55^{0}C

M	T (K)	PCO2e	a expt	a calc	Error %
3.46	328	15.4	0.269	0.2107	21.67286
		30.11	0.365	0.2844	22.08219
		203	0.705	0.5863	16.83688
		393	0.795	0.7026	11.62264
		838	0.881	0.8177	7.185017

Table 7: Predicted Carbon Dioxide solubilities at 3.46M in 70^{0}C

M	T (K)	PCO2e	a expt	a calc	Error %
	343	8.92	0.125	0.1146	8.32
		32.12	0.248	0.2111	14.87903
		133	0.45	0.3909	13.13333
		301	0.618	0.5291	14.38511
		603	0.739	0.6551	11.35318
		855	0.778	0.7163	7.930591
		1013	0.813	0.7445	8.425584

Table 8: Predicted Carbon Dioxide solubilities at 3.46M in 80^{0}C

M	T (K)	PCO2e	a expt	a calc	Error %
	353	9.22	0.074	0.0928	25.40541
		29.32	0.14	0.1631	16.5
		174	0.351	0.3631	3.447293
		389	0.509	0.4955	2.652259
		754	0.641	0.6162	3.868955

Table 9: Predicted Carbon Dioxide solubilities at 3.46M in 90^{0}C

M	T (K)	PCO2e	a expt	a calc	Error %
	363	3.27	0.03	0.0441	47
		47.31	0.139	0.1665	19.78417
		207.8	0.299	0.3269	9.331104
		522.8	0.474	0.4734	0.126582
		867.8	0.561	0.5655	0.802139

4. Mol: 4.28M

Temperature: 40^0C

Table 10: Predicted Carbon Dioxide solubilities at 4.28M in 40^0C

M	T (K)	PCO2e	a expt	a calc	Error %
4.28	313	15.4	0.269	0.2584	3.94052
		30.11	0.365	0.3437	5.835616
		203	0.705	0.6613	6.198582
		393	0.795	0.768	3.396226
		838	0.881	0.8635	1.986379

Mol: 4.28M

Temperature: 50^0C

Table 11: Predicted Carbon Dioxide solubilities at 4.28M in 55^0C

M	T (K)	PCO2e	a expt	a calc	Error %
	328	8.92	0.125	0.1391	11.28
		32.12	0.248	0.2518	1.532258
		133	0.45	0.4513	0.288889
		301	0.618	0.5944	3.81877
		603	0.739	0.7158	3.139378
		855	0.778	0.7713	0.861183
		1013	0.813	0.7961	2.078721

Mol 4.28M

Temperature: 70^0C

Table 12: Predicted Carbon Dioxide solubilities at 4.28M in 70^0C

M	T (K)	PCO2e	a expt	a calc	Error %
	343	9.22	0.074	0.0987	33.37838
		29.32	0.14	0.1723	23.07143
		174	0.351	0.3783	7.777778
		389	0.509	0.5119	0.569745
		754	0.641	0.6316	1.466459

Mol: 4.28M

Temperature: 80^0C

Table 13: Predicted Carbon Dioxide solubilities at 4.28M in 80^0C

M	T (K)	PCO2e	a expt	a calc	Error %
	353	3.27	0.03	0.0467	55.66667
		47.31	0.139	0.1737	24.96403
		207.8	0.299	0.3377	12.94314
		522.8	0.474	0.4851	2.341772
		867.8	0.561	0.5766	2.780749

Mol: 4.28M

Temperature: 100^0C

Table 11: Predicted Carbon Dioxide solubilities at 4.28M in 100^0C

M	T (K)	PCO2e	a expt	a calc	Error %
	373	0.88	0.009	0.0153	70
		11.87	0.037	0.0577	55.94595
		159	0.142	0.2059	45
		519	0.274	0.3494	27.51825
		824	0.351	0.4221	20.25641

APPENDIX IV: Validation of solubilities in 35wt% of MDEA with Haji Sulaiman's model

wt%	T	PCO2 (kPa)	αexp (molCo2/molMDEA)	αcalc1(molCo2/molMDEA)	Error %	αcalc2(molCo2/molMDEA)	Error %
35	29.85	1.064	0.114	0.112	1.75	0.1772	55
	303	3.13	0.244	0.234	4.1	0.2884	16.4
		4.802	0.333	0.3	9.91	0.3456	3.78
		10.535	0.483	0.452	6.42	0.4687	2.96
		29.756	0.673	0.691	2.67	0.6498	3.44
		48.37	0.793	0.799	0.76	0.7294	8.02
		95.83	0.88	0.905	2.84	0.8222	9.17
	39.85	1.064	0.103	0.091	11.65	0.1361	32.14
	313	3.069	0.197	0.177	10.15	0.2241	13.75
		5.176	0.267	0.243	8.99	0.2833	16.58
		10.029	0.374	0.353	5.61	0.3745	0.134
		30.349	0.603	0.585	2.99	0.5608	7
		47.52	0.688	0.698	1.45	0.6406	6.88
		93.956	0.805	0.837	3.98	0.753	6.46
	49.85	0.997	0.079	0.065	17.72	0.1018	28.86
	323	2.938	0.148	0.133	10.14	0.1721	16.28
		4.761	0.194	0.18	7.22	0.216	11.34
		9.725	0.298	0.275	7.72	0.2979	0.134
		28.435	0.471	0.483	2.55	0.4608	2.16
		44.136	0.59	0.585	0.85	0.5381	9.645
		91.154	0.726	0.752	3.58	0.6683	7.94
				Average Error	5.859524	Average error	12.28919

APPENDIX V: Validation of solubilities in 50wt% of MDEA with Haji Sulaiman's model

wt%	T	PCO2 (kPa)	αexp (molCo2/molMDEA)	αcalc1(molCo2/molMDEA)	Error %	αcalc2(molCo2/molMDEA)	Error %
50	29.85	0.0099	0.027	0.014	48.15	0.0109	59.62963
	303	0.984	0.061	0.067	9.84	0.0984	61.31148
		4.918	0.149	0.185	24.16	0.2095	40.60403
		9.853	0.284	0.276	2.82	0.2848	0.28169
		29.509	0.516	0.48	6.98	0.4421	14.32171
		49.1	0.633	0.601	5.06	0.5281	16.57188
		98.2	0.761	0.758	0.39	0.6491	14.70434
	39.85	0.095	0.015	0.011	26.67	0.013	13.33333
	313	0.954	0.052	0.049	5.77	0.0732	40.76923
		4.762	0.086	0.136	58.14	0.127	47.67442
		9.523	0.19	0.207	8.95	0.2186	15.05263
		28.521	0.384	0.391	1.82	0.351	8.59375
		47.535	0.513	0.495	3.51	0.4288	16.41326
		95.234	0.654	0.653	0.15	0.547	16.36086
	49.85	0.09	0.01	0.007	30	0.0084	16
	323	0.901	0.037	0.035	5.41	0.046	24.32432
		4.514	0.084	0.103	22.62	0.097	15.47619
		9.028	0.151	0.159	5.3	0.165	9.271523
		27.084	0.251	0.308	22.71	0.3437	36.93227
		45.139	0.363	0.4	10.19	0.4205	15.84022
		90.279	0.516	0.548	6.2	0.5376	4.186047
				Average Error	14.51619	Average Error	23.22156

APPENDIX V: Validation of solubilities in 35wt% of MDEA with Jou et al model

wt%	T	PCO2 (kPa)	αexp (molCo2/molMDEA)	αcalc1(molCo2/molMDEA)	Error %
35	25	0.001	0.005	0.0078	56
	298.15	0.00688	0.0166	0.0185	11.44578
		0.0218	0.0329	0.0316	3.951368
		0.0295	0.0402	0.0365	9.20398
		1.55	0.334	0.2391	28.41317
		4.22	0.452	0.3665	18.91593
		9.26	0.638	0.4925	22.80564
		181	1.025	0.9821	4.185366
		698	1.146	1.0123	11.66667
		2040	1.308	1.236	5.504587
		3550	1.479	1.375	7.031778
		4570	1.587	1.487	6.301197
		5260	1.676	1.5504	7.494033
		6380	1.833	1.7499	4.533552
					197.4531
	70	0.00208	0.0009	0.00087	3.333333
	343.15	0.00335	0.00129	0.0013	0.775194
		0.048	0.0056	0.0133	137.5
		0.305	0.0208	0.0239	14.90385
		0.951	0.0439	0.0505	15.03417
		40.9	0.369	0.3659	0.840108
		447	0.841	0.7807	7.170036
		993	1.011	0.8807	12.88823
		2320	1.147	0.9421	17.86399
		2730	1.182	0.9496	19.66159
		4230	1.235	1.154	6.558704
		6020	1.397	1.223	12.45526
					248.9845
	120	0.0725	0.00124	0.00133	7.258065
	393.15	0.116	0.00166	0.00184	10.84337
		3.84	0.0133	0.0145	9.022556
		57.7	0.0973	0.112	15.10791
		493	0.336	0.4515	34.375
		1930	0.7203	0.7203	0
		3380	0.91	0.8912	2.065934
		4660	1.043	1.0672	2.32023
		5490	1.152	1.1887	3.185764
				Average Error	16.58176