A COMPARISON STUDY OF DIFFERENT EMPIRICAL MODELLING METHODS IN PREDICTING CO_2 SOLUBILITY IN DIETHANOLAMINE, N-METHYLDIETHANOLAMINE AND THEIR MIXTURES

by

MOHD FAREEZ AKMAL BIN MOHD FADZLI

Dissertation submitted in partial fulfilment of the requirement for the
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CERTIFICATION OF APPROVAL

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Chemical Engineering Programme

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Approved by,

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UNIVERSITI TEKNOLOGI PETRONAS

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MAY 2013

CERTIFICATION OF ORIGINALITY

This is to certify that I, Mohd Fareez Akmal Bin Mohd Fadzli (I/C No : 901103-13-6217), 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.

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MOHD FAREEZ AKMAL BIN MOHD FADZLI

ABSTRACT

Acid gas removal from natural gas, synthesis gas and refinery gas stream is very important in plant industry to prevent corrosion in the subsequent piping and as per requirement by various organizations and companies. Because of the corrosiveness of H_2S and CO_2 the sales gas is required to be sweetened to contain no more than a quarter grain H_2S per 100 standard cubic feet (4 parts per million) and to have a heating value of no less than 920 to 980 Btu/SCF, depending on the contract. The most widely used process to remove acid gas from natural gas is by using alkanlomines, and of the alkanolamines the most common are n-methyldiethanolamine (MDEA) and diethanolamine (DEA).

In this study, data from Khalid Osman et al (2012), A. Benamor et al (2005) and Zhang et al (2002) will be used to simulate the solubility of CO_2 in DEA and MDEA mixtures using Multiple Linear Regression (MLR) and Artificial Neural Network (ANN) and the performance will be compared to show which model is better for CO_2 absorption. Furthermore, data from Jou et al (1982) and Lee et al (1972) will be used to study the solubility of CO_2 in pure DEA and MDEA aqueous solution and simulation of the models will be compared between the models and the reference research works mentioned earlier.

MLR has proved it cannot be used to predict CO_2 for pure DEA, MDEA and their mixtures. The results clearly shown that the model is pressure dependent as it has large coefficient compared to other parameters which is very small and becomes dominant in the equation thus neglecting them in predicting the CO_2 loading data. ANN proved the model can be used to predict CO_2 solubility in the alkanolamines and their mixtures. Developed model for DEA and MDEA mixture has an absolute relative deviation δ_{AAD} 10.47 % while for data from Khalid Osman et al (2012), A. Benamor et al (2005) and Zhang et al (2002) are 17.06%, 12.09% and 9.82% respectively. In pure alkanolamines prediction, ANN model of CO2 solubility predicted in pure DEA has δ_{AAD} 4.02% while from the experimental data of A. Benamor et al (2005) has absolute relative deviation of 4.72%. As for prediction of CO_2 in pure MDEA, the model resulted δ_{AAD} of 9.77% compared to the reference paper from A. Benamor et al (2005) with 10.76%.

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First and foremost, I would like to express my praises to God for His blessing in completing this thesis. Special appreciation and sincere gratitude is extended to my supervisor, Ir Dr Abdul Halim Shah Maulud for patience, motivation, enthusiaism and immense knowledge to guideand support me during these two semester sessions to complete this project.

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CHAPTER 1

INTRODUCTION

1.1 Background Study

The oil and gas production industry has multiplied and become one of the important industry from around the globe. For decades to come, gas will be the energy source of choice to meet worldwide environmental standards. Fortunately gas reserves are growing; but new gas is often found to be of substandard quality in remote and / or stranded areas of the world.

Raw natural gases contain mainly different types of hydrocarbon as well as contaminants. The acid gas, which often refer to carbon dioxide (CO_2) and hydrogen sulfide (H_2S) is what makes the acid gas. Thus, the raw natural gases needs to be treated in order to remove the acid gas.

Dry carbon dioxide (CO_2) is inert and is commonly used as an industrial material. However, CO_2 is an acidic gas when it reacts with water to form carbonic acid (Informative guide for CO_2). Carbonic acid corrosion is a formidable challenge and its effect on carbon steels has been recognized for years as a major source of damage in oil field equipment and gas pipelines. Hence, the formation of carbonic acid and moisture

will decrease pipeline flow capacities, even resulting in blockages, and potential harm to valves, filters and compressors that are being used throughout the process.

The separation of CO_2 and H_2S from natural gas is called gas sweetening. Gas sweetening is one of the important purification processes which is employed to remove acidic contaminants from natural gases prior to sale. One of the most common method yet effective and economic to separate CO_2 is absorption by using aqueous solutions of alkanolamines. Although various processes have been proposed for such processed, the gas absorption method with different solvents is widely used.

Alkanolamine is broadly classified into primary, secondary and tertiary depending on the number of alkyl group(s) attached to the nitrogen atom in the molecule structure. Monoethanolamine(MEA), diethanolamine (DEA) and n-methyldiethanolamine (MDEA) are such of the examples. While the CO_2 absorption rate of the primary and secondary amines such as MEA and DEA is high, in the case of tertiary amines such as TEA and MDEA, the CO_2 absorption rate is considerably lower. Thanks to low carbamate stability, the CO_2 absorption capacity of the tertiary amine aqueous solutions is high and due to the formation of stable carbamate, the primary and secondary amines have low capacity of CO_2 absorption (Guevara F.M.,1998)

Sterically hindered amines such as 2-Amino-2-Methyl-1-Propanol (AMP) could be a primary amine in which the amino group is attached to a tertiary carbon atom or a secondary amine in which the amino group is attached to secondary or tertiary carbon atoms (Sartori G., 1983). These amines have high capacity absorption and absorption rate as well as selectivity and degradation resistance. Since equilibrium data are indispensable for design of gas absorption units, many researchers have reported the solubility of acid gases in various types of amines. Solubility of CO_2 in MEA, DEA and MDEA aqueous solutions at various temperatures, amine concentrations and pressures has been reported. Jane et al.(1997) determined the solubility of CO_2, H_2S and their mixtures in the system of DEA+AMP aqueous solution. Teng et al.(1989) measured the solubility of acid gases in AMP at 50^oC and 3.43 $kmol/m^3$ AMP. Roberts et al. (1988) reported the solubility of acid gases in AMP.

Several model has been developed to analyze the solubility of CO_2 in aqueous solution of alkanolamine and to correlate the solubility data such as Kent-Eisenberg (KE), Modified Kent-Eisenberg (M-KE), Electrolyte-NRTL, Extended Debye-Hückel (E-DH), Pitzer and Li-Mather models were proposed to correlate the solubility data. Kent & Eisenberg(1976) modeled the solubility of acid gases and their mixtures in MEA and DEA aqueous solutions. They considered equilibrium constants of carbamate formation and protonation of these amines to be temperature-dependent only. Since the KE model is an empirical model, in a wide range of temperature, pressure and amine concentrations it cannot properly predict the solubility of acid gases in amine aqueous solutions.

Although the KE equilibrium constant of carbamate formation was used in this work, the new correlations forMEA and DEA equilibrium constant of protonationreaction were presented.To increase the accuracy of predicting the solubilityof acid gases in amines, the activity coefficients mustbe considered. To do so, Deshmukh et al.(1981)and Pitzeret al.(1973, 1974)proposed the E-DH and Pitzer models,respectively. It should be noted that application of thesemodels would be more complicated than that of the K-Eand M-KE. In the Pitzer, E-DH and Li-Mather models theactivity coefficients were expressed in terms of longas well as short-range intermolecular forces.

The above models are based on the first principles model. Another type of modelling is using the empirical model technique. The disadvantage of using first principle model are the model is complex and time consuming. However, the advantages of using empirical model are the time is significantly reduced, less complex for on-line optimization, less time required to develop the model and it is easy to identify from input-output data. Among the empirical models are Multiple Linear Regression and Artificial Neural Network.

A multiple linear regression analysis is carried out to predict the values of adependent variable, *Y*, given a set of p explanatory variables (x1,x2,….,x*p).* In multiple linear regression, there are p explanatory variables, and the relationshipbetween the dependent variable and the explanatory variables is represented by the following equation:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_p x_{pi} + e_i$$

Where:

β_0 is the constant term and

β_1 to β_p are the coefficients relating the p explanatory variables to the variables of interest.

Thus, multiple linear regression can be thought of an extension of simple linear regression, where there are p explanatory variables, or simple linear regression can be thought of as a special case of multiple linear regression, where p=1. The term 'linear' is used because in multiple linear regression assumption has been made that y is directlyrelated to a linear combination of the explanatory variables.

An artificial neural network (ANN) is a powerful modelling method in various scientific fields. The capability of learning from experimental results and the simplicity of implementation are the main advantages of the ANN over other mathematical modelling methods.

1.2 Problem Statement

Before designing plant or pipeline in the large scale, the need to run simulation that replicate the process of the plant based on the actual parameters is really important as to predict the scenario. Hence, the modelling of the CO_2 solubility in the amines is also important. By doing a model for the CO_2 solubility, predicting the result for the actual process based on the modelling can be studied and further improved before implementing in the actual process. As the solubility of CO_2 is highly non-linear [16], a nonlinear modelling technique is required in order to get accurate result. In this study, several empirical modelling techniquessuch as Multiple Linear Regression (MLR) and Artificial Neural Network (ANN)will be investigated to model the CO_2 solubility in DEA and MDEA system.

1.3 Objectives

1. To compile the equilibrium data of CO_2 solubility in aqueous solutions of DEA, MDEA and their mixtures.
2. To develop a model for CO_2 solubility in DEA, MDEA and their mixtures using MLR and ANN modelling techniques.
3. To analyze the predicted CO_2 loading data in each of the modelling methods compared to the experimental data.
4. To compare the performance of the predicted CO_2 loading data for each techniques.

1.4 Scope of Study

In this study, the main focus are:

1. The alkanolamines used are diethanolamine (DEA), n-methyldiethanolamine (MDEA) and their mixtures. This does not include the mixtures of the said chemicals with promoter such as piperazine (PZ).
2. Modelling technique to be used are Multi Linear Regression (MLR) and Artificial Neural Network (ANN).
3. The tool to be used for modelling is Matrix Laboratory (MATLAB) software.

CHAPTER 2

LITERATURE REVIEW

2.1 Carbon Dioxide

Carbon dioxide comprises two oxygen atoms covalently bonded to a single carbon atom, with an O-C-O angle of 180°. As such it is very stable, no process other than photosynthesis having been discovered that is able effectively to reduce carbon dioxide to carbon monoxide. Carbon dioxide is not classified by the UN as toxic(United Nations, 2007).

CO_2 is a colourless, odourless gas found within the earth's atmosphere. It is the product of combustion and of respiration and is also utilised in the process of photosynthesis in plants. It has an interesting property in that it sublimes or changes from a solid (it freezes at −78 °C) directly into a gas at atmospheric pressure, without first becoming a liquid. This is why it is sometimes referred to as 'dry ice'. CO_2 is produced commercially for use in fizzy drinks, dry cleaning and in de-caffeinating coffee. It can be transported or stored in liquid form, but only when held at a very high pressure.

Carbon dioxide gas is colourless, heavier than air (1 521 times as heavy, with a density of about 1,98 g/litre), has a slightly irritating odour, and freezes at −78,5 °C to form carbon dioxide snow. Carbon dioxide cannot exist as a liquid at atmospheric pressure. At a pressure of anything above 5,11 bar(a) and at a temperature between −56,6 °C and 31,1 °C it becomes liquid (see Figure 2.1), and its density rises with temperature to 1 180 kg/m^3. The liquid/gas equivalent (1,013 bar and 15 °C (per kg of solid)) is 845 vol/vol. If the temperature of liquid carbon dioxide drops below 56,6 °C it becomes solid (see Figure 2.1). Solid carbon dioxide usually has a snow-like appearance, and can be compressed into blocks to form ‘dry ice’. Solid CO_2 will form in

vessels/pipelines when conditions fall below the triple point and this may not be snow-like.

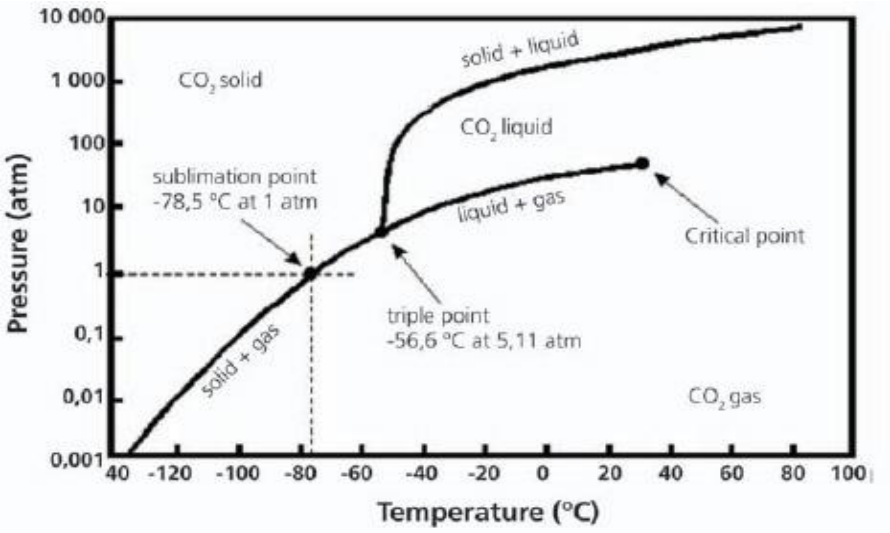

Figure 2.1: Pressure-Temperature phase diagram for CO_2

The triple point (at a pressure 5,11 bar and temperature of −56,7 °C) is defined as the temperature and pressure where three phases (gas, liquid and solid) can exist simultaneously in thermodynamic equilibrium. The solid-gas phase boundary is called the sublimation line, as a solid changing state directly into a gas is called sublimation. Physically, this boundary implies that the gas and solid can co-exist and transform back and forth without the presence of liquid as an intermediate phase.

Above the critical point (73,8 bar and 31,1 °C), the liquid and gas phases cannot exist as separate phases, and liquid phase carbon dioxide develops supercritical properties, where it has some characteristics of a gas and others of a liquid.

A phase diagram, as shown in Figure 2.1 is a common way to represent the various phases of a substance and the conditions under which each phase exists. However, it tells us little regarding how the changes of state for carbon dioxide occur during a transient.

CO_2 is considered to be the most important of the greenhouse gases. With human activity, CO_2 is emitted into the atmosphere whenever organic matter burned as fuel.

The carbon in the organic matter reacts with air to produce CO_2 and energy. The largest sources of CO_2 are fossil fuel powered power stations (those that use coal, oil or gas) and petrol or diesel powered transport (most cars and lorries).

Known as acid gas, CO_2 has to be removed from natural gas to avoid problems such as corrosion equipment plugging due to the formation of CO_2 solid in the low temperature system and also reducing the heating value of natural gas. CO_2 have to be eliminated from the natural gas to increase the heating value and fulfill the product demand specification. The process of removing CO_2 and H_2S from natural gas is known as gas treating or gas sweetening. The gas sweetening process refers to the removal of the sour odour of the gas from the sulphur in H_2S.Acid gases (CO2 and H2S) are the main impurities in natural gas. Acid gases are corrosive to the pipeline and have a very low heating value.

2.2 Alkanolamine

Alkanolamines are chemical compounds that carry hydroxy (-OH) and amino (-NH_2, -NHR, and -NR_2) functional groups on an alkane backbone. Alkanolamine is broadly classified into primary, secondary and tertiary depending on the number of alkyl group(s) attached to the nitrogen atom in the molecule structure. Monoethanolamine (MEA), diethanolamine (DEA) and n-methyldiethanolamine (MDEA) are such of the examplesrespectively as well as sterically hindered amines such as 2-Amino-2-Methyl-1-Propanol (AMP).

2.3 Methyldiethanolamine (MDEA)

Methyldiethanolamine is a clear, colorless or pale yellow liquid with ammonical odor. It is miscible with water, alcohol and benzene. Methyldiethanolamine is also known as a MDEA or n-Methyldiethanolamine. Methyldiethanolamine is widely used as a decarbonizer and sweetening agent in chemical, oil refinery, gas synthesis, natural gas & gas. MDEA is more efficient absorber then MEA & DEA for sulphur contains impurity and acid gases found in natural gas processing.

MDEA is versatile bifunctional molecules compound that combines the characteristic of Amine and hydroxyl group. Thus, during the reaction it behaves like alcohol and amine group but amine group usually exhibits the greater activities. MDEA can be modified with the help of some additives, the product is known as an Activated Methyl Diethanolamine.

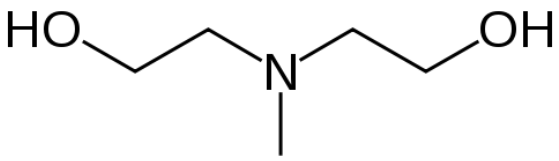

Figure 2.2: Molecular structure of MDEA

MDEA is considered moderately irritating to the eyes, but only slightly irritating to the skin. The product is not corrosive under the conditions of the corrositivity test and is not regulated as a hazardous material for transportation purposes. Because of the low vapour pressure of MDEA, exposure to vapours is not expected to pose significant hazard under normal workplace conditions (Huntsman, 2007).

SPECIFICATION :	METHYL DIETHANOLAMINE
METHYL DIETHANOLAMINE - MDEA Content (% Wt.)	**99 (Minimum)**
Chemical Formula	**CH3N (C2H4OH)**
Specific Gravity at 20/20`C.	**1.040 - 1.044**
Distillation Range (760 mm/Hg.) : I.B.P.	**242`C. (Minimum)**
: D.P.	**260`C. (Maximum)**
Moisture	**0.2- 0.5%**
Colour	**150 APHA (Maximum)**
Refractive Index at 20`C	**1.4694**
Viscosity at 20`C	**101 CPS (Approx.)**
Flash Point (pmcc)	**135°C (Approx.)**
Equivalent Mass	**118 -121**
Cas No.	**105-59-9**

Figure 2.3: Specification and properties of MDEA

MDEA is widely used as an absorption solvent of removing acid gases in sweetening gas process, because of it possesses the characteristic such as higher hydrogen sulphide selectivity, bigger absorption capacity, lower regeneration energy, smaller hot degradation and lesser corrosive.

2.4 Diethanolamine (DEA)

Diethanolamine, often abbreviated as DEA or DEOA, is an organic compound with the formula $HN(CH_2CH_2OH)_2$. This colorless liquid is polyfunctional, being a secondary amine and a diol. Like other organic amines, diethanolamine acts as a weak base. Reflecting the hydrophilic character of the alcohol groups, DEA is soluble in water, and is even hygroscopic. Amides prepared from DEA are often also hydrophilic.

Diethanolamine is produced by reacting ethylene oxide with ammonia. In most production facilities, ethylene oxide and ammonia are reacted in a batch process that yields a crude mixture of ethanolamine, diethanolamine and triethanolamine. The mixture is then distilled to separate and purify the individual compounds(Edens MR et al, 2004).

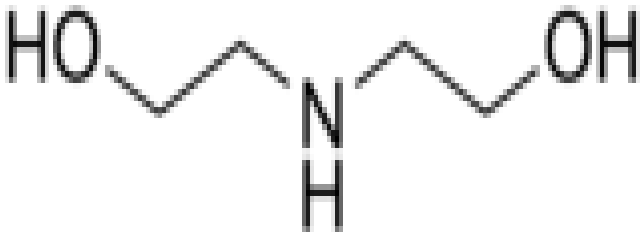

Figure 2.4: Molecular structure of DEA

The reaction of ethylene oxide with aqueous ammonia first produces ethanolamine:

$$C_2H_4O + NH_3 \rightarrow H_2NCH_2CH_2OH$$

which reacts with a second and third equivalent of ethylene oxide to give DEA and triethanolamine:

$$C_2H_4O + H_2NCH_2CH_2OH \rightarrow HN(CH_2CH_2OH)_2$$

$C_2H_4O + HN(CH_2CH_2OH)_2 \rightarrow N(CH_2CH_2OH)_3$

DEA is used as a surfactant and a corrosion inhibitor. It is used to remove hydrogen sulfide and carbon dioxide from natural gas. In oil refineries, DEA in water solution is commonly used to remove hydrogen sulfide from various process gases. It has an advantage over a similar amine ethanolamine in that a higher concentration may be used for the same corrosion potential. This allows refiners to scrub hydrogen sulfide at a lower circulating amine rate with less overall energy usage.

Diethanolamine helps to overcome the limitation of MEA, and can be used in the present of COS and CS2. Operating with solutions containing 25-30% by weight of DEA can be used to process natural gas with even high acid gases content.

DEA is considered to be chemically stable; DEA can be heated to its normal boiling point (269 ^{o}C at 760 mmHg) before decomposition. Therefore reduce the solvent degradation during stripping and reduce solvent loss and accumulation in the unit.

The heat of reaction of DEA with CO_2 is low compared to other amines hence the heat generated in the absorber during CO_2 absorption process is low which increases the solvent loading in the absorber as solubility or loading of CO_2 increases at low temperature.

2.5 Multiple Linear Regression (MLR)

A multiple linear regression analysis is carried out to predict the values of a dependent variable, *Y*, given a set of p explanatory variables (x1, x2,….,x*p)*. In multiple linear regression, there are p explanatory variables, and the relationship between the dependent variable and the explanatory variables is represented by the following equation:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_p x_{pi} + e_i$$

Where:

β_0 is the constant term and

β_1 to β_p are the coefficients relating the p explanatory variables to the variables of interest. So, multiple linear regression can be thought of an extension of simple linear regression, where there are p explanatory variables, or simple linear regression can be thought of as a special case of multiple linear regression, where p=1. The term‘linear’ is used because in multiple linear regression assumption has been made that y is directly related to a linear combination of the explanatory variables. MLR is one of the most used methods for forecasting. Thismethod is widely used to fit the observed data and to createmodels that can be used for the prediction in many researchfields.

When explanatory variables are correlated with each other, the application of this method usually presents some drawbacks due to the fact that high correlations between predictor variables can difficult a correct analysis. The dependence of the explanatory variables can be removed through the application of principal component analysis (PCA). PCA creates new variables, the principal components (PC), that are orthogonal and uncorrelated. These variables are linear combinations of the original variables. The PC are ordered in such a way that the first component has the largest fraction of the original data variability(Abdul-Wahab et al, 2005).

2.6 Artificial Neural Network

Artificial neural networks are inspired by the early models of sensory processingby the brain. An artificial neural networkcan be created by simulating a network ofmodel neurons in a computer. By applyingalgorithms that mimic the processes of realneurons, we can make the network ‘learn’ tosolve many types of problems. A model neuronis referred to as a threshold unit and itsfunction is illustrated in Figure 2.5(a). It receivesinput from a number of other units or externalsources, weighs each input and adds themup. If the total input is above a threshold,the output of the unit is one; otherwise it iszero. Therefore, the output changes from 0 to 1 when the total weighted sum of inputsis equal to the threshold. The points in inputspace satisfying this condition define a socalledhyperplane. In two dimensions, ahyperplane is a line, whereas in three dimensions,it is a normal plane. Points on one sideof the hyperplaneare

classified as 0 and thoseon the other side as 1. It means that a classificationproblem can be solved by a thresholdunit if the two classes can be separated by ahyperplane. Such problems, as illustrated inthree dimensions in Figure 2.5(b) , are said to belinearly separable.

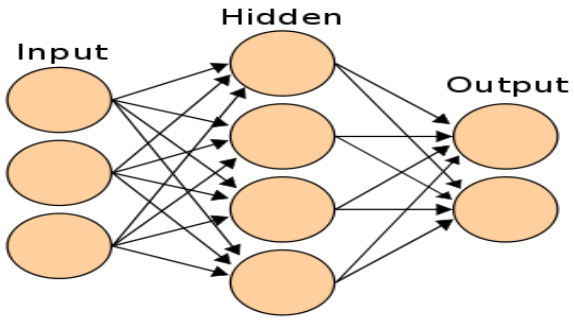

Figure 2.5: An artificial neural network is an interconnected group of nodes, replicating to the vast network of neurons in the human brain.

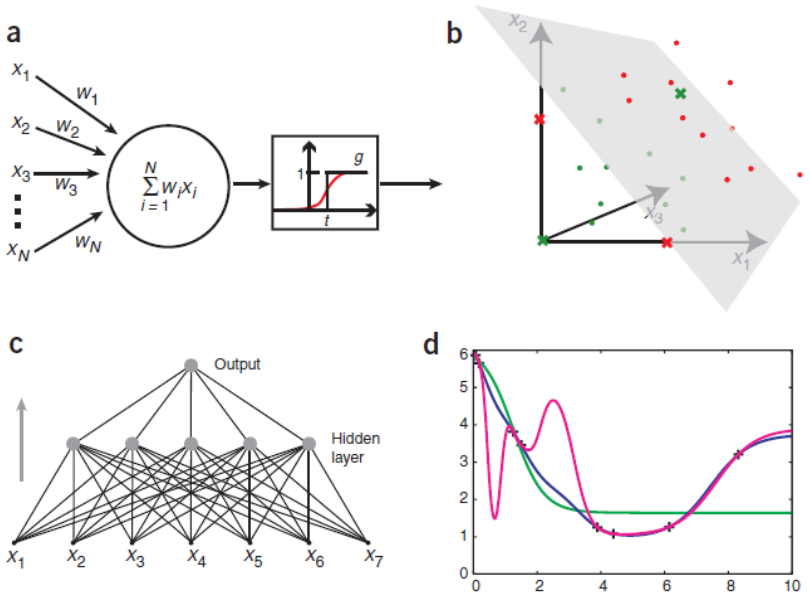

Figure 2.6Artificial neural networks

Figure 2.6 (a) shows graphical representation of the McCulloch-Pitts model neuron or threshold unit. The threshold unit receives input from *N* other units or external sources, numbered from 1 to *N*. Input *i*is called $x_i$and the associated weight is called w_i. The total input to a unit is the weighted sum over all inputs, $\sum_{i=1}^{N} w_i\, x_i = w_1 x_1 +$

$w_2x_2 + \ldots + w_Nx_N$. If this were below a threshold *t*, the output of the unit would be 1 and 0 otherwise. Thus, the output can be expressed as $g(\sum_{i=1}^{N} w_1x_1 - t$, where g is the step function, which is 0 when the argument is negative and 1 when the argument is nonnegative (the actual value at zero is unimportant; here, we chose 1). The so-called transfer function, *g*, can also be a continuous sigmoid as illustrated by the red curve.

Figure 2.6 (b) explains linear separability. In three dimensions, a threshold unit can classify points that can be separated by a plane. Each dot represents input values x_1, $x_2$and $x_3$to a threshold unit. Green dots correspond to data points of class 0 and red dots to class 1. The green and red crosses illustrate the 'exclusive or' function—it is not possible to find a plane (or a line in the x_1, $x_2$plane) that separates the green dots from the red dots.

Figure 2.6 (c) shows a feed-forward network. The network shown takes seven inputs, has five units in the hidden layer and one output. It is said to be a two-layer network because the input layer does not perform any computations and is not counted.

An over-fitting graph is shown in Figure 2.6 (d). The eight points shown by plusses lie on a parabola (apart from a bit of 'experimental' noise). They were used to train three different neural networks. The networks all take an *x* value as input (one input) and are trained with a *y* value as desired output. As expected, a network with just one hidden unit (green) does not do a very good job. A network with 10 hidden units (blue) approximates the underlying function remarkably well. The last network with 20 hidden units (purple) over-fit the data; the training points are learned perfectly, but for some of the intermediate regions the network is overly creative.

Neural networks have been applied to many interesting problems in different areas of science, medicine and engineering and in some cases, they provide state-of-the-art solutions. Neural networks have sometimes been used haphazardly for problems where simpler methods would probably have given better results, giving them a somewhat poor reputation among some researchers.

CHAPTER 3

METHODOLOGY

3.1 Project Methodology

3.1.1 Reference data

The first phase of the project is to collect all the data needed in order to calculate the CO_2 solubility in the said alkanolamines. The data such as concentration of MDEA, DEA and their mixtures, CO_2 partial pressure and temperature which is the crucial parameters for developing the models is obtained from various sources mostly from the past research works. During the study, the parameters of data based on the Table 3.1.

Author	**Temperature (K)**	**Partial pressure CO_2**	**DEA**	**MDEA**	**Mixtures**
HjSulaiman et al. (1998)	303,313,323	0.1 – 104 kPa	/	/	
A.Benamor et al. (2005)	303-323	0.09-100 kPa			/
Khalid et al (2012)	362.1, 392.1, 412.1	500 – 1500 kPa			/
Zang et al. (2002)	313,323,333,343	1 – 95 kPa			/

Table 3.1: The reference data used as the parameters

3.1.2 Multiple Linear Regression

The next stage of the project is to develop the MLR and ANN models. Throughout this study, matrix laboratory (MATLAB) software will be used to develop the models. Let $y = \alpha$ (α is being the CO_2 solubility), then a proposed matrix for linear equation such that

$$X = \begin{bmatrix} Partial\ pressure(X_1) & Temperature\ (X_2) & Concentration(X_3) \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ (X_j) & (X_k) & (X_l) \end{bmatrix}$$

And for multiple linear regression, the proposed matrix

$$X_m = \begin{bmatrix} X_1 & X_2 & X_3 & X_1^2 & X_2^2 & X_3^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ X_j & X_k & X_l & X_m & X_n & X_o \end{bmatrix}$$

The multiple linear regression equation that can be derived such that

$$\alpha = aT + bP + cC + dT^2 + eP^2 + fC^2 + g$$

The command **LM = LinearModel.fit(X,y,'linear')** for linear expression and **LM = LinearModel.fit(X,y,'quadratic')** for quadratic expression is used in MATLAB software in order to regress the model with respect to X and y values. The objective is to find the value of the estimates as the coefficient of the parameters x1, x2 and x3 which are CO_2 partial pressure, temperature and concentration of DEA, MDEA or ratio of the concentration of DEA and MDEA respectively and also to determine which of the parameters should be removed based on the p-value obtained. If the p-value is less than 0.05, the parameter is kept and vice versa.

The model then needs to be re-regress containing only the values which are kept for p-value < 0.05. New matrix needs to be construct consist of the parameters which are

to be kept in the first regression. The regression process will be repeated until the p-values is less than 0.05.

For the second form of the MLR model, all the parameters are kept the same except for temperature that will be using 1/T instead. This is to further study if the model can determine the CO_2 solubility using different form of parameter, which in this case is 1/T.

For developing the ANN model, the first step is by randomizing the input data. All the data from the reference papers will be randomize and divided into three parts:

1. 65% of data will be used for training the neuron.
2. 10% of data will be used for validation.
3. 25% of data will be used for testing the neuron.

The trial and error method will then be used to determine number if nodes for the neuron. Every number of neuron will give different results in term of Mean Square Error (MSE) and Regression. The trial and error process will be perform by setting the number of nodes as 1 and the results will then be collected. Number of nodes will be increase to 3, 5, 7, 9, 15, 20, 25, 30 and up to 35. The result from each iteration will be recorded and number of nodes that show lowest MSE and highest Regression wil be the optimal number of nodes for the ANN model. The basis of this model is that MSE equals to zero which means no error and Regression equals to one means no deviation of generated output data from the targeted data.

All the data will be trained and tested based on the input and the target data which the CO_2 is loading from the experimental data. The generated output will then be simulated with the network that has the optimal number of neurons that have been identified earlier together with the input parameters. The command used to simulated the output data is **sim(network,input).** The calculated CO_2 loading data is the result from the simulated output data.

3.1.3 Model Assessment

Before concluding the outcome of the project, the error analysis on the results need to calculate by comparing the generated CO_2 loading with the experimental data from the reference papers. Error calculated in the form of average absolute relative deviation percent, δ_{AAD} using the following equation:

$$(\delta_{AAD}) = \frac{\sum_{i=1}^{N} \frac{|\alpha_{calc} - \alpha_{exp}|}{\alpha_{exp}}}{N} \times 100\%$$

Where

α_{calc} = generated CO_2 loading

α_{exp} = experimental CO_2 loading

N = number of data points

The summary of the methodology is shown in Figure 3.1.

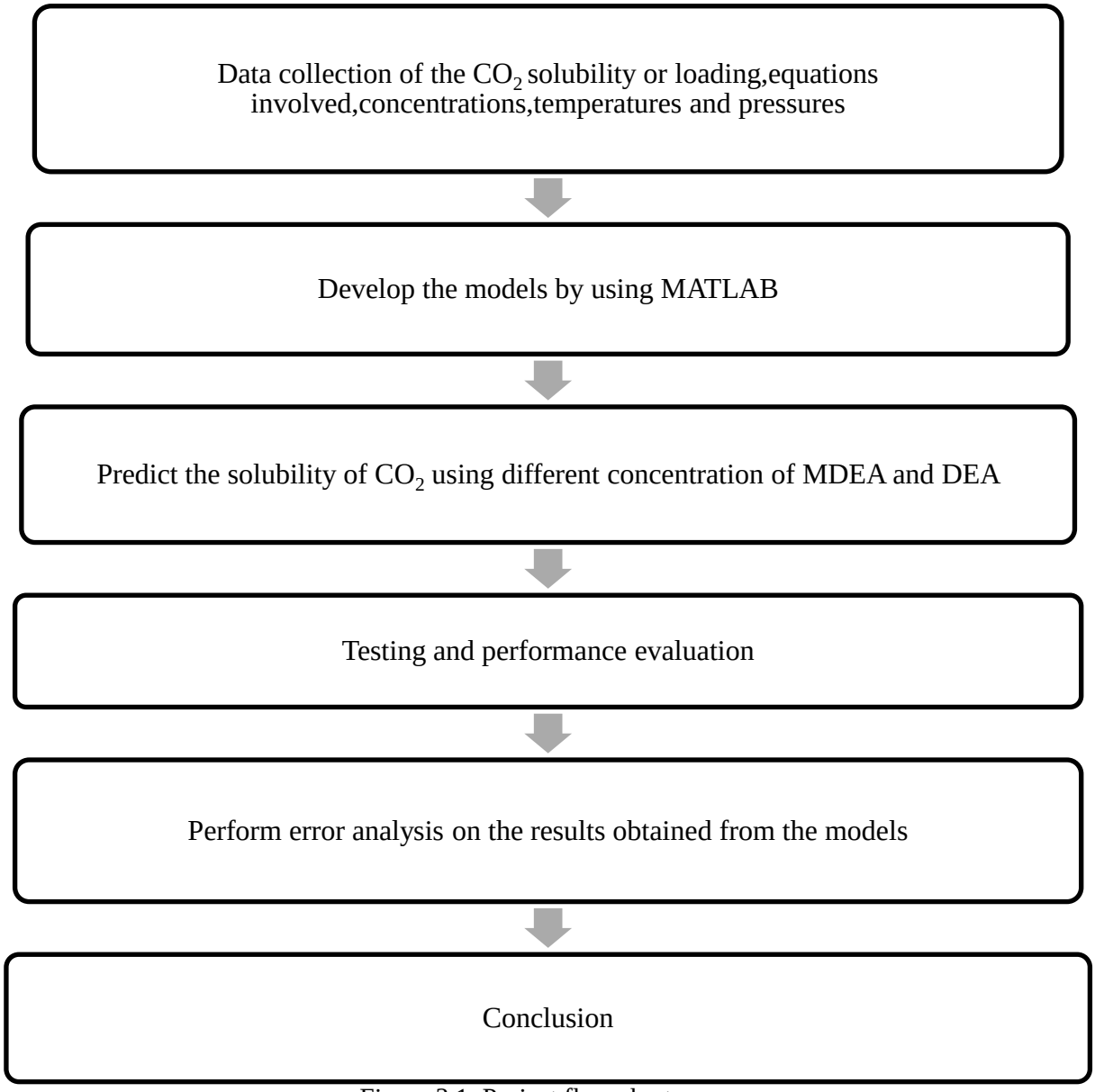

Figure 3.1: Project flow chart

3.2 Gantt Chart

Table 3.1 explains the timelines for Final Year Project II (FYPII) that will be done in this semester. Several objectives are expected to be achieved during the end of FYPII.

The first third weeks of the semester is allocated for the student to finalize the data of parameters and starts to develop the Multiple Linear Regression (MLR) model. Then the next task in starting week 4 is to develop the MLR model by using different forms of the parameters that is planned until week 6.

The result is then need to be finalized during week 6 and week 7. Further thorough data analysis will be performed during week 6 until week 9. The generated CO_2 loading data from the model and from the experimental data will be compared to analyze the error analysis.

After that, the data will be compiled all together during week 6 until week 10. Further task is to identify appropriate solution and recommendation to improve the result of the model for week 10 until week 12. Week 13 and week 14 are planned to finalize the data and the result.

Activities/Plan	**Final Year Project II (FYPII)**													
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Finalizing data of parameters and developing MLR and ANN models														
Develop different forms of parameters for the models														
Finalizing the result of the model														
Performing data analysis between the model data and the experimental data														
Compile all data together														
Identify appropriate solution and recommendation for improving the result of the models														
Finalize all data and result														
Key Milestones	**Final Year Project II (FYPII)**													
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Thorough data analysis and interpretation														
Completion of FYP Technical Paper														
Final Year Project Oral Presentation														
Submission of Project Dissertation (Hard Bound)														

Table 3.2: Gant Chart of FYP II

CHAPTER 4

RESULT AND DISCUSSION

In this section, the result of the modesl that has been complete so far will be shown and discussed. By using experimental data from Zhang et al(2002), A Benamour et al (2005) and Khalid et al(2012) for mixture of DEA and MDEA, the models have been developed.

4.1 Multiple Linear Regression of Pure DEA

4.1.1 Linear Regression

Estimated Coefficients:

	Estimate	**SE**	**tStat**	**pValue**
(Intercept)	24.644	9.7942e-08	2.5162e+08	1.9915e-283
x1	33.592	9.9658e-08	3.3707e+08	3.9891e-288
x2	-2.2469e-15	1.0071e-07	-2.2311e-08	1
x3	2.5576e-15	1.0033e-07	2.5493e-08	1

Table 4.1: Linear regression result for pure DEA

4.1.2 Quadratic Regression

Estimated Coefficients:

	Estimate	**SE**	**tStat**	**pValue**
(Intercept)	24.644	4.2618e-07	5.7825e+07	4.3973e-219
x1	33.592	4.1662e-07	8.063e+07	1.4707e-223
x2	-2.6819e-15	2.2528e-07	-1.1905e-08	1
x3	-1.2769e-15	2.2082e-07	-5.7825e-09	1
x1:x2	-3.1776e-16	2.4248e-07	-1.3105e-09	1
x1:x3	3.2376e-15	2.3106e-07	1.4012e-08	1
x2:x3	-1.269e-15	2.3777e-07	-5.3371e-09	1
x1^2	3.5275e-16	2.5777e-07	1.3685e-09	1

x2^2	-1.6841e-15	2.9235e-07	-5.7608e-09	1
x3^2	0	0	NaN	NaN

Table 4.2: Quadratic regression result for pure DEA

4.2 Multiple Linear Regression of Pure MDEA

4.2.1 Linear Regression

Estimated Coefficients:

	Estimate	**SE**	**tStat**	**pValue**
(Intercept)	8.6707e-14	4.6864e-06	1.8502e-08	1
x1	1	3.9598e-09	2.5254e+08	1.7403e-283
x2	-2.4119e-16	1.4859e-08	-1.6231e-08	1
x3	1.4738e-15	1.2029e-07	1.2251e-08	1

Table 4.3: Linear regression result for pure MDEA

4.2.2 Quadratic Regression

Estimated Coefficients:

	Estimate	**SE**	**tStat**	**pValue**
(Intercept)	0	0	NaN	NaN
x1	1	0	Inf	0
x2	-3.0239e-14	0	-Inf	0
x3	3.4763e-12	0	Inf	0
x1:x2	-1.5146e-17	0	-Inf	0
x1:x3	-2.4012e-17	0	Inf	0
x2:x3	3.0914e-16	0	Inf	0
x1^2	6.7584e-19	0	-Inf	0
x2^2	4.781e-17	0	Inf	0
x3^2	-5.9515e-13	0	-Inf	0

Table 4.4: Quadratic regression result for pure MDEA

4.3 Multiple Linear Regression of Mixture of DEA and MDEA

4.3.1 Linear Regression

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	1.5719e-13	0	Inf	0
x1	1	0	Inf	0
x2	-4.8422e-16	0	-Inf	0
x3	-1.8782e-15	0	-Inf	0

Table 4.5: Linear regression result for mixture of DEA and MDEA

4.3.2 Quadratic Regression

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	-4.8226e-12	0.00033751	-1.4289e-08	1
x1	1	2.2692e-07	4.4069e+06	0
x2	3.0518e-14	2.1579e-06	1.4143e-08	1
x3	7.6219e-14	6.8729e-06	1.109e-08	1
x1:x2	1.4353e-18	7.1878e-10	1.9969e-09	1
x1:x3	2.8773e-17	4.5109e-09	6.3786e-09	1
x2:x3	-2.3776e-16	2.1755e-08	-1.0929e-08	1
x1^2	2.1172e-19	1.7945e-10	1.1798e-09	1
x2^2	-4.8377e-17	3.4488e-09	-1.4027e-08	1
x3^2	-1.0303e-15	2.8108e-07	-3.6656e-09	1

Table 4.6: Quadratic regression result for mixture of DEA and MDEA

From all the result presented in the table, shows that the loading data is dominant to x1, which is the CO_2 partial pressure. This is because only x1 exhibit coefficient of 1, which is too big and become dominant in the equation. Other parameters show estimates with value too small. This would assume that other parameters has no significant contribution in the equation compared to the partial pressure. This would also conclude that the equation is in function of the partial pressure as it become dominant and others has coefficient too small to be considered in the equation.

4.4 Multiple Linear Regression of Pure DEA (1/T)

4.4.1 Linear Regression

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	24.644	1.3851e-07	1.7792e+08	7.383e-278
x1	33.592	1.4092e-07	2.3838e+08	1.471e-282
x2	1.4257e-15	1.4237e-07	1.0014e-08	1
x3	-4.4247e-15	1.4184e-07	-3.1194e-08	1

Table 4.7: Linear regression result for pure DEA

4.4.2 Quadratic Regression

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	24.644	4.2732e-07	5.7671e+07	4.7775e-219
x1	33.592	4.1642e-07	8.0668e+07	1.449e-223
x2	2.812e-15	2.2325e-07	1.2596e-08	1
x3	-2.2832e-15	2.2066e-07	-1.0347e-08	1
x1:x2	5.6915e-15	2.4131e-07	2.3586e-08	1
x1:x3	-2.8411e-15	2.3057e-07	-1.2322e-08	1
x2:x3	-1.9409e-15	2.3681e-07	-8.1959e-09	1
x1^2	1.497e-16	2.5772e-07	5.8089e-10	1
x2^2	-2.086e-15	2.9474e-07	-7.0775e-09	1
x3^2	0	0	NaN	NaN

Table 4.8: Quadratic regression result for pure DEA

4.5 Multiple Linear Regression of Pure MDEA (1/T)

4.5.1 Linear Regression

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	25.193	1.3851e-07	1.8188e+08	3.2683e-278
x1	30.859	1.4109e-07	2.1872e+08	3.5539e-281

x2	1.686e-15	1.4089e-07	1.1967e-08	1
x3	-3.7026e-15	1.4058e-07	-2.6338e-08	1

Table 4.9: Linear regression result for pure MDEA

4.5.2 Quadratic Regression

Estimated Coefficients:

	Estimate	**SE**	**tStat**	**pValue**
(Intercept)	25.193	3.4424e-07	7.3183e+07	2.9663e-222
x1	30.859	2.9733e-07	1.0379e+08	5.866e-227
x2	2.9903e-15	1.7097e-07	1.749e-08	1
x3	-2.3774e-15	1.6986e-07	-1.3996e-08	1
x1:x2	2.4267e-15	1.8924e-07	1.2823e-08	1
x1:x3	1.4515e-15	1.7797e-07	8.1555e-09	1
x2:x3	-3.2334e-15	1.7441e-07	-1.8539e-08	1
x1^2	5.3138e-15	1.9211e-07	2.766e-08	1
x2^2	6.214e-15	2.3952e-07	2.5944e-08	1
x3^2	0	0	NaN	NaN

Table 4.10: Quadratic regression result for pure MDEA

4.6 Multiple Linear Regression of Mixture of DEA and MDEA (1/T)

4.6.1 Linear Regression

Estimated Coefficients:

	Estimate	**SE**	**tStat**	**pValue**
(Intercept)	27.118	1.2549e-07	2.1609e+08	0
x1	34.003	1.2627e-07	2.6928e+08	0
x2	-6.6671e-16	1.2624e-07	-5.2812e-09	1
x3	-5.918e-15	1.263e-07	-4.6856e-08	1

Table 4.11: Linear regression result for mixture of DEA and MDEA

4.6.2 Quadratic Regression

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	-3.6044e-13	0.00018135	-1.9875e-09	1
x1	1	1.1974e-07	8.3514e+06	0
x2	2.2826e-10	0.11329	2.0148e-09	1
x3	3.7671e-14	3.6792e-06	1.0239e-08	1
x1:x2	-1.0858e-12	3.7525e-05	-2.8935e-08	1
x1:x3	-2.9026e-17	2.4112e-09	-1.2038e-08	1
x2:x3	-1.1112e-11	0.0011374	-9.7694e-09	1
x1^2	3.582e-18	9.5931e-11	3.7339e-08	1
x2^2	-3.638e-08	17.692	-2.0563e-09	1
x3^2	-5.5345e-16	1.5024e-07	-3.6837e-09	1

Table 4.12: Quadratic regression result for mixture of DEA and MDEA

4.7 Artificial Neural Network of Mixture DEA and MDEA

Net	Neuron	MSE (Training)	Regression (Training)	MSE (Validating)	Regression (Validating)	MSE (Testing)	Regression (Testing)
1	1	0.0254397	0.691581	0.0184513	0.884589	0.0232636	0.541711
2	3	0.045492	0.201336	0.0226305	0.709831	0.0514549	0.115710
3	5	0.0055930	0.944118	0.00544034	0.947366	0.0167729	0.777367
4	7	0.00324365	0.961991	0.00574389	0.940929	0.115413	0.494238
5	9	0.0120171	0.868242	0.0131435	0.822890	0.0301576	0.591231
6	15	0.0174990	0.791978	0.0158619	0.811450	0.0164552	0.815500
7	20	0.0142303	0.841923	0.0171880	0.838953	0.0149020	0.823227
8	25	0.0105900	0.871120	0.0129695	0.808179	0.0148009	0.873302
9	30	0.00729455	0.918009	0.0143475	0.839814	0.0438370	0.601202
10	35	0.0105105	0.887976	0.0328929	0.694506	0.0243187	0.682179

Table 4.13: Simulation Results

From the results above, network 8 with 25 neurons is selected as the best optimal result which shown the least MSE and highest R values for testing. Further analysis is illustrated in the graph below

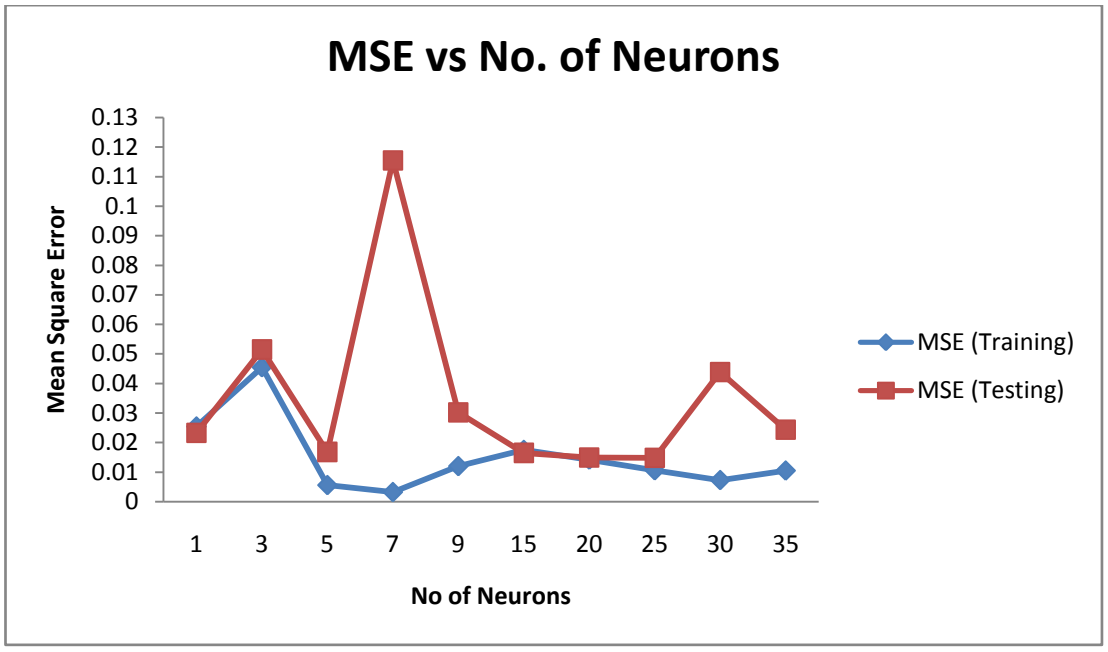

Figure 4.1: Graph MSE vs No of Neurons

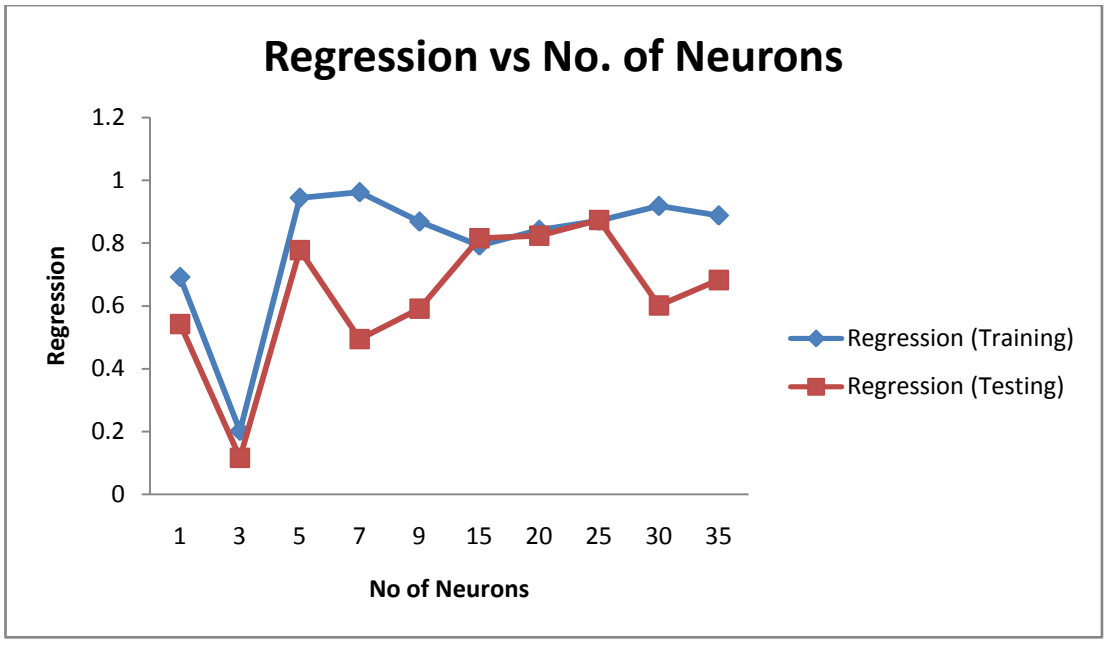

Figure 4.2: Graph regression vs No of Neurons

Based on the graphs, for this neural network model, the optimal neuron can be obtained at 5 neurons, which the model would give the minimum MSE and maximum value of R.

Besides MSE and Regression, there are also generated output data as a part of the results. The output data was simulated as a result of the training and testing by the neurons. However, there are small deviations between the generated output data and the target data. Generated output and calculated error are tabulated in the Appendix. Error is calculated using this equation:

$$Error = Target\ data - Output\ data$$

Deviations between generated and experimental data of the CO2 loading were plotted in the graphs. Results were divided into 6 parts based on the concentration of amines:

1. 1.5M MDEA + 0.5M DEA
2. 1.0M MDEA + 1.0M DEA
3. 0.5M MDEA + 1.5M DEA
4. 3.0M MDEA + 1.0M DEA
5. 2.0M MDEA + 2.0M DEA
6. 1.0M MDEA + 3.0M DEA

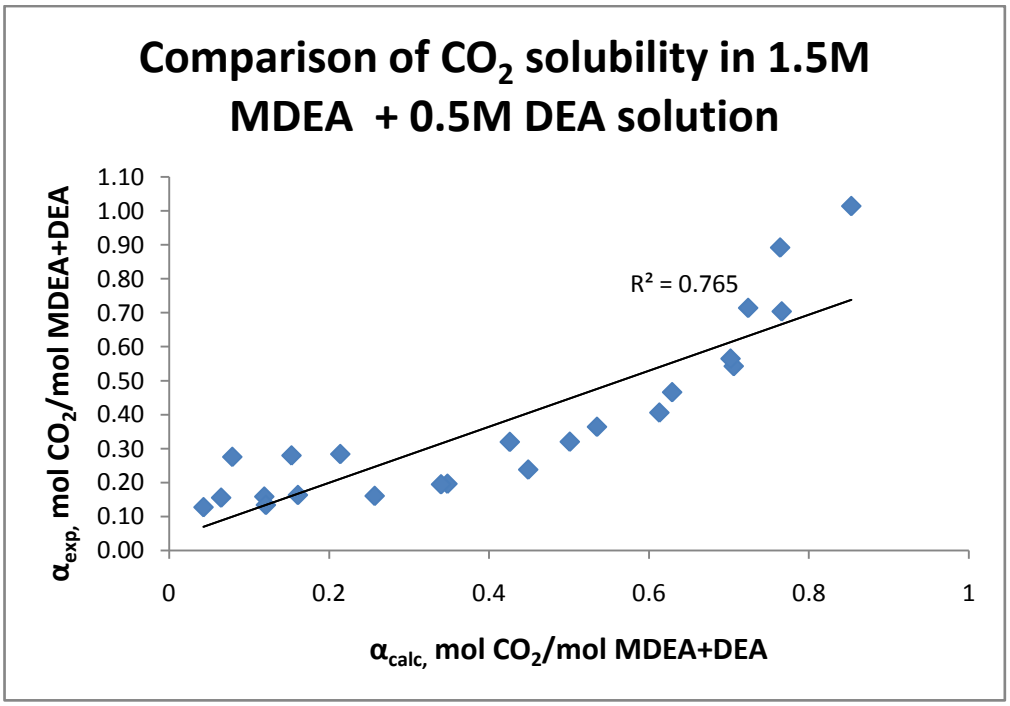

Figure 4.3 Comparison of CO_2 solubility in 1.5M MDEA + 0.5M DEA solution

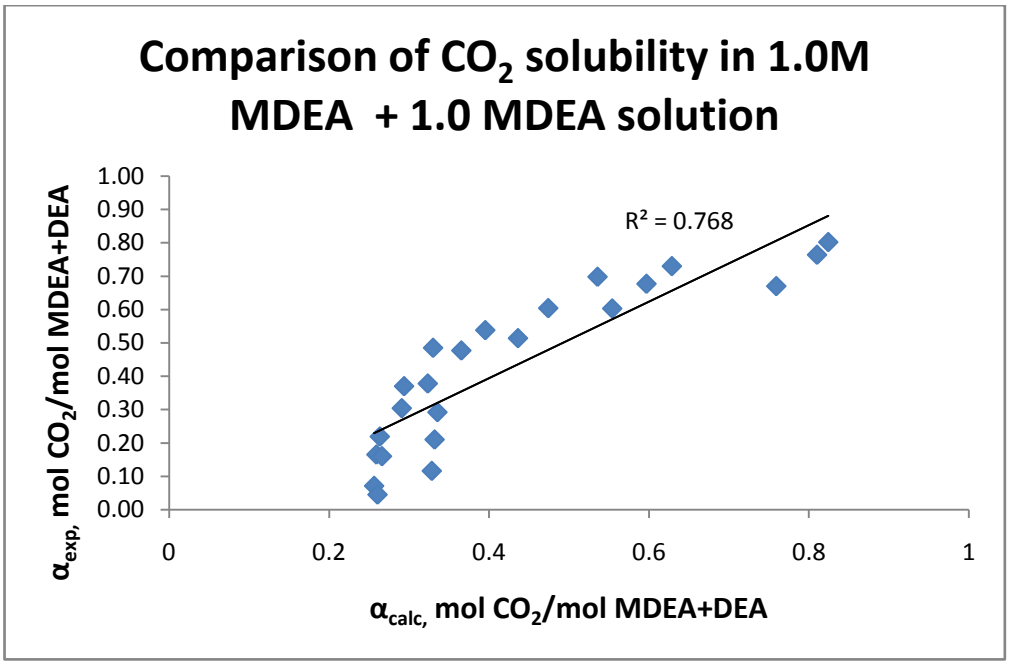

Figure 4.4 Comparison of CO_2 solubility in 1.0M MDEA + 1.0 MDEA solution

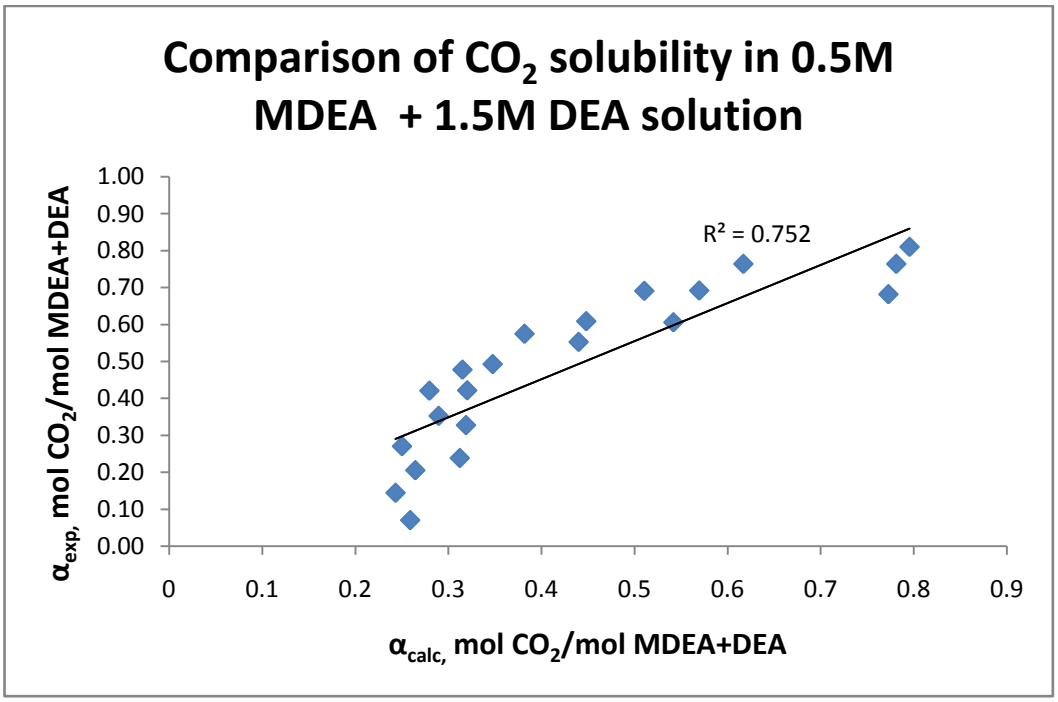

Figure 4.5 Comparison of CO_2 solubility in 0.5M MDEA + 1.5M DEA solution

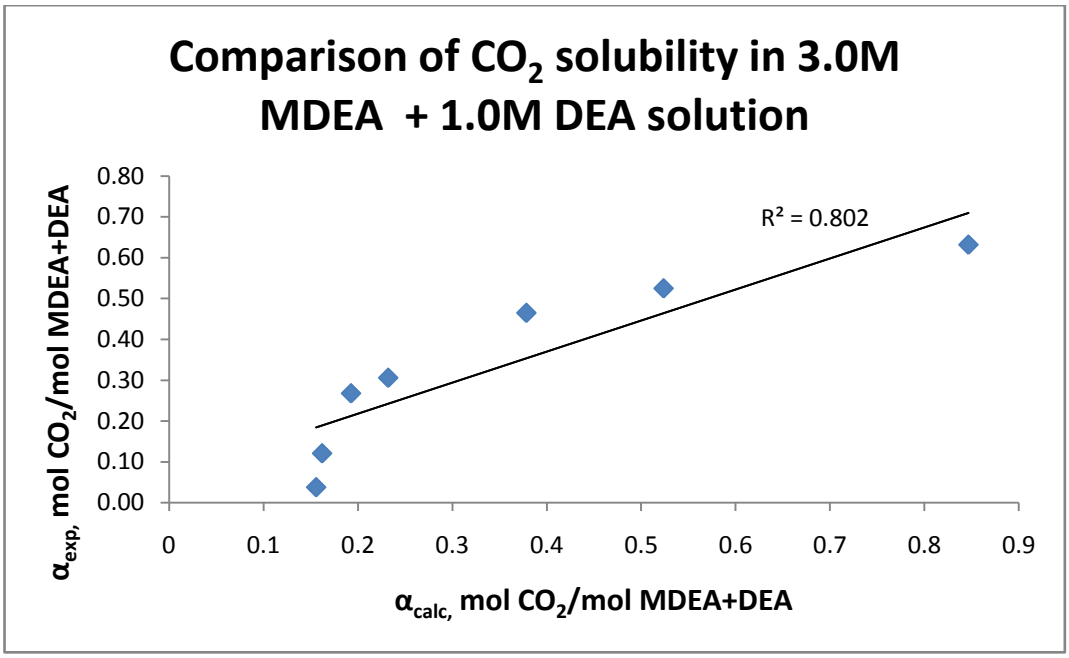

Figure 4.6 Comparison of CO_2 solubility in 3.0M MDEA + 1.0M DEA solution

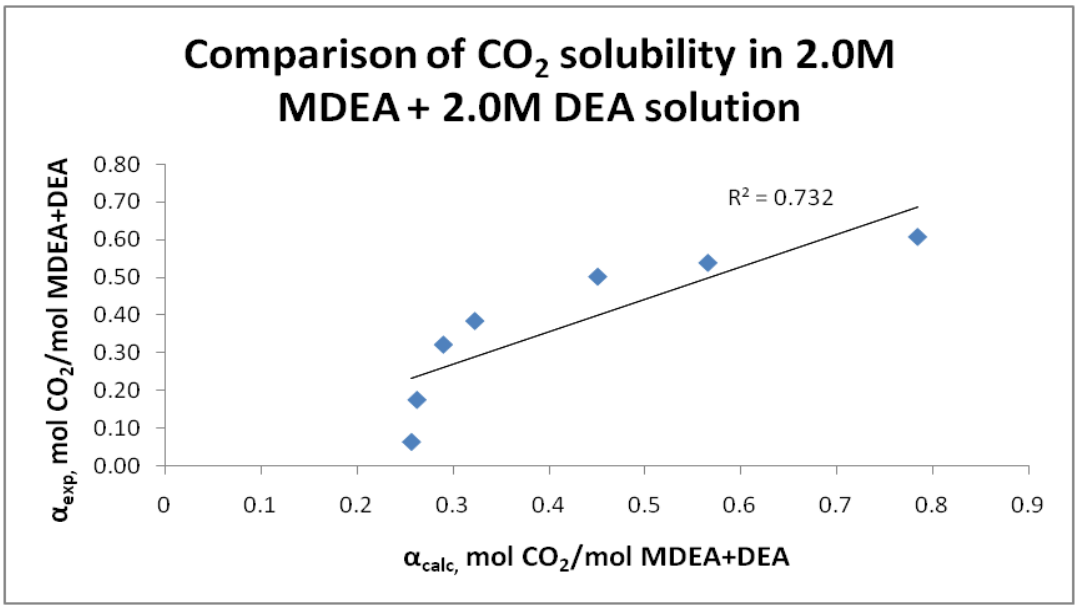

Figure 4.7 Comparison of CO_2 solubility in 2.0M MDEA + 2.0M DEA solution

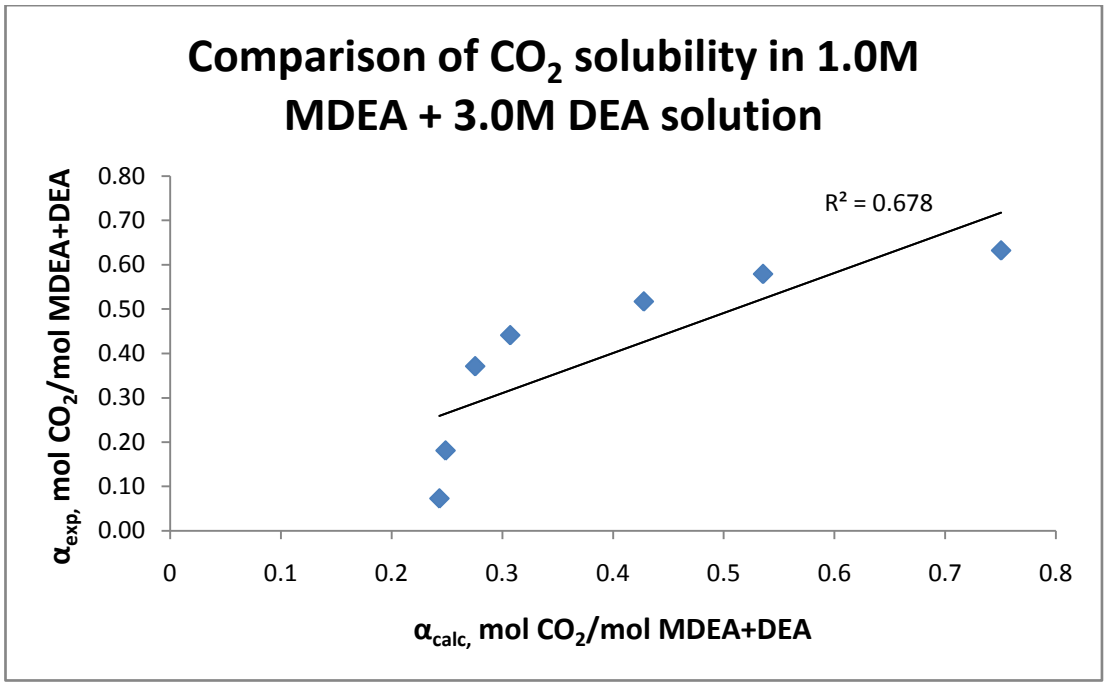

Figure 4.8 Comparison of CO_2 solubility in 1.0M MDEA + 3.0M DEA solution

From the graph, all the generated data followed the same pattern as experimental data with the presence of some deviation. The deviation however, is small since proved by the average absolute relative deviation percent δ_{AAD} calculated which is 10.47% while for data from Khalid Osman et al (2012), A. Benamor et al (2005) and Zhang et al (2002) are 17.06%, 12.09% and 9.82% respectively. From the value of δ_{AAD} the model is considered as valid and has the ability to predict CO_2 solubility in MDEA and DEA mixture since the deviation is smaller compared to the previous works that have been done before.

4.8 Artificial Neural Network of Pure DEA and Pure MDEA

In this method, only pure DEA and pure MDEA is used in each of the prediction method. The concentrations for both amines used are 2.0M and 4.0M respectively. Comparison of generated data and experimental data of CO_2 loading are plotted in the graphs.

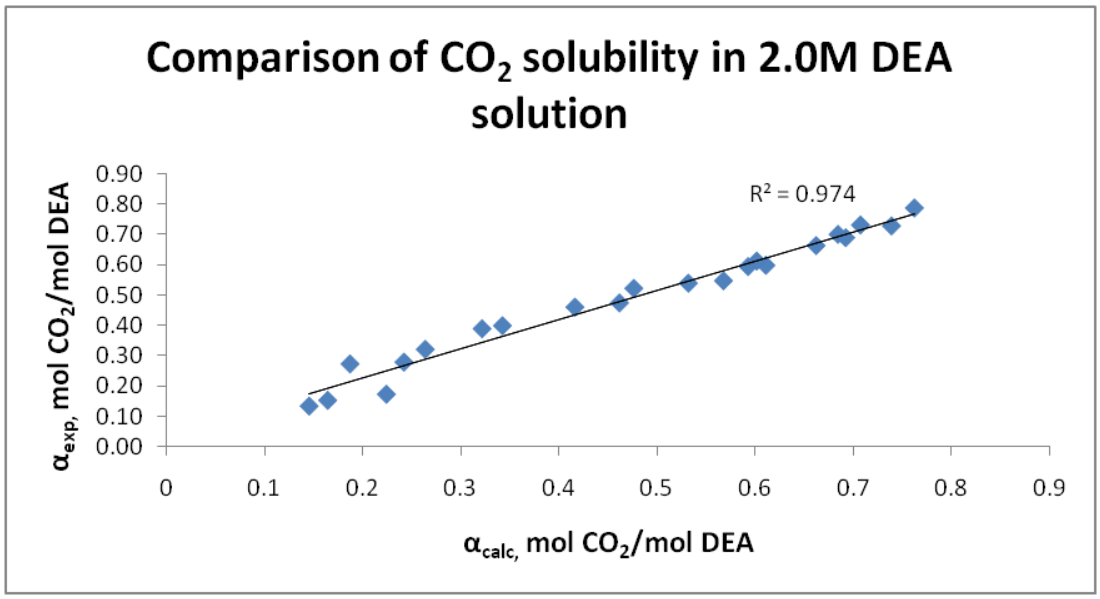

Figure 4.9 Comparison of CO_2 solubility in 2.0M DEA solution

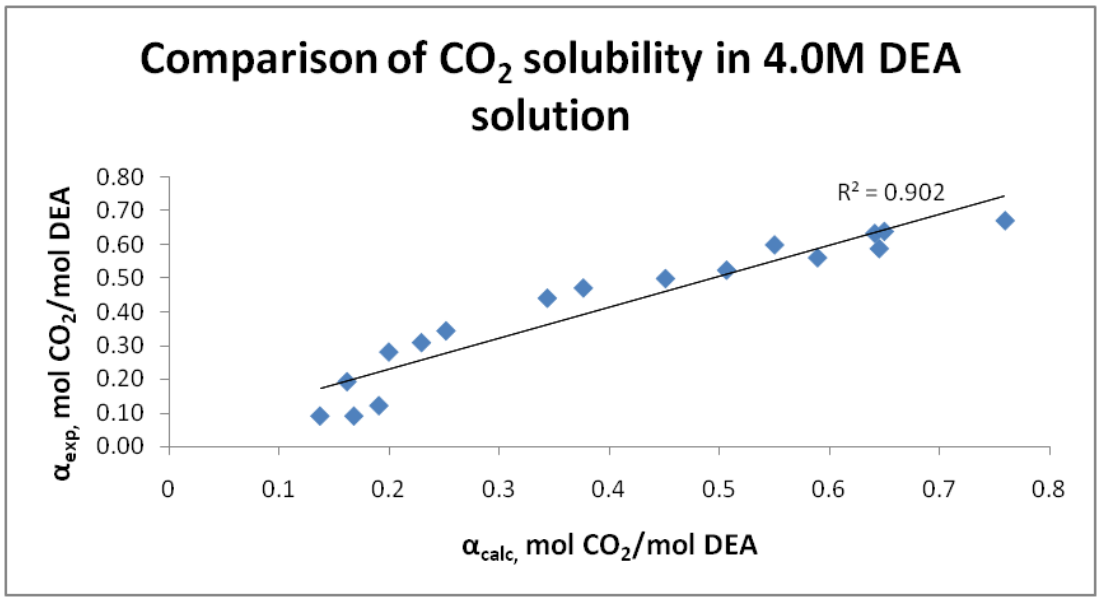

Figure 4.10 Comparison of CO_2 solubility in 4.0M DEA solution

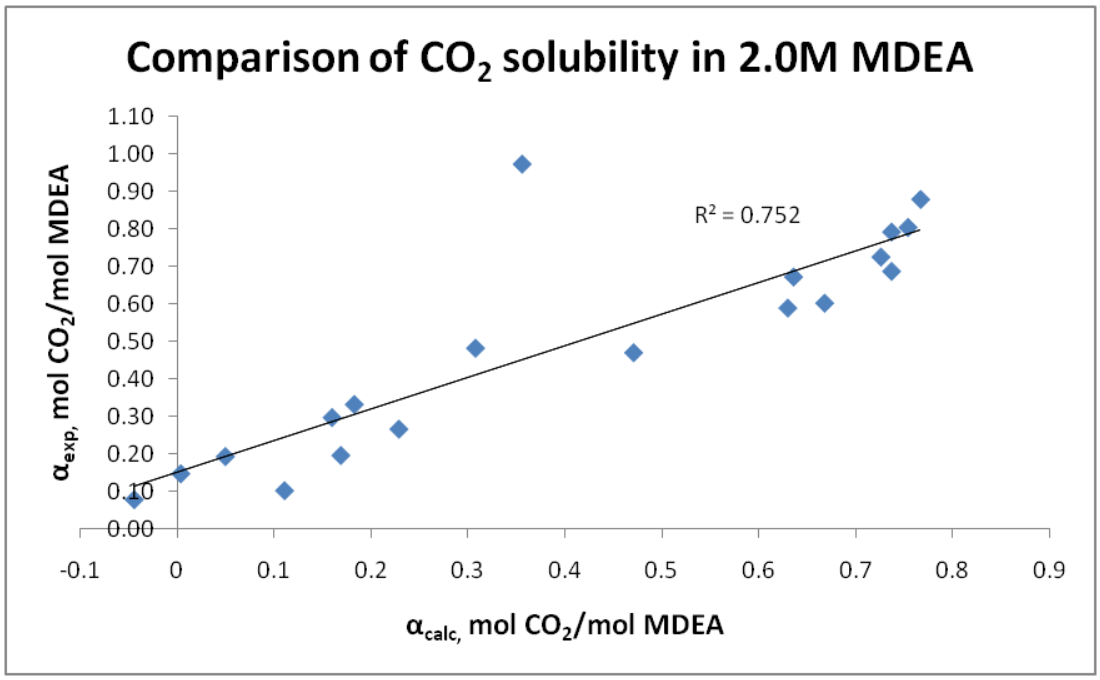

Figure 4.11 Comparison of CO_2 solubility in 2.0M MDEA

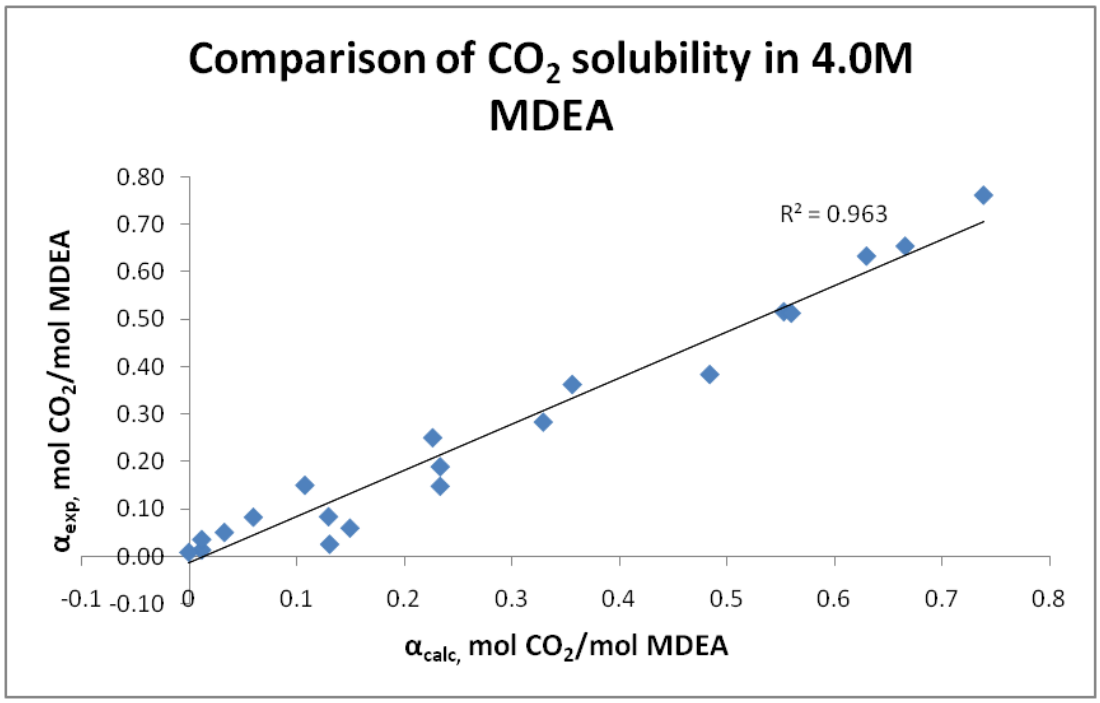

Figure 4.12 Comparison of CO_2 solubility in 4.0M MDEA

In pure alkanolamines prediction, ANN model of CO2 solubility predicted in pure DEA has δ_{AAD} 4.02% while from the experimental data of A. Benamor et al (2005) has absolute relative deviation of 4.72%. As for prediction of CO_2 in pure MDEA, the model resulted δ_{AAD} of 9.77% compared to the reference paper from A. Benamor et al (2005) with 10.76%.

The error or deviations are small since new models were developed for each method. ANN models can learn the pattern from data input and the accuracy and precision were great as the deviations are small.

CHAPTER 5

CONCLUSION

The study of this project conclude that the MLR models still can be used to study the CO_2 solubility in MDEA,DEA and their mixture. From the result as discussed in Chapter 4, it can be concluded that the equation is pressure dependent. This can be seen from the result as x1 has large value that it becomes dominant in the equation, neglecting other parameters. This proved that Multiple Linear Regression cannot be used to predict CO_2 solubility in pure DEA, MDEA and their mixtures.

On the other hand, Artificial Neural Network, the overall performance of the model was great as long as it is given chance to train and validate data the input data. This can be proven by the $\boldsymbol{\delta_{AAD}}$ of the developed models which are smaller compared to the previous works. Since ANN was developed by learning the input data as well as the patterns of the inputs, it cannot interpret the data once the new input does not happen to have same pattern with the precious input.

As the conclusion, Multiple Linear Regression cannot be used to predict CO2 solubility in pure DEA, MDEA and their mixtures. ANN has great ability to predict CO_2 solubility in pure DEA, MDEA and their mixtures only by developing models for each situation and condition due to the limitation of ANN itself which cannot simulate the new input data if they do not have the same patterns with the previous model developed.

There are some recommendations that can be applied in order to improve the mathematical system. Firstly, by adding more experimental data to the system so that the neural network model can learn the patterns of the output more accurate and precise. Secondly, by using various forms of parameters, MLR might be able to predict CO_2 solubility under those the conditions.

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APPENDICES

Appendix I

```
% Mixture DEA and MDEA MLR

% by fareez 16/8/2013


%Data Input


X=zeros(158,3);


% CO2 Partial Pressure (kPa)


X(:,1)=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2
28.9 50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0
10.3 29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1
10.2 31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5
47.4 95.1 4.81 6.10 8.40 9.61 11.80 16.80 21.40 25.20 29.80 9.01 11.0 14.50 17.10 23.50
33.80 39.10 44.50 49.00 17.90 18.40 21.80 22.8 33.1 40.10 51.2 57.3 64.1 72.1 21.8 29.0
40.80 48.2 55.2 61.0 63.50 12.1 15.2 18.9 37.7 42.8 14.6 19.0 27.4 35.5 46.1 56.8 150.00
450.00 105.100 351.00 61.00 149.00 151.00 450.00 1153.00 49.00 160.00 351.00 450.0
1050.0 152.00 57.00 351.00 152.00 153.00 1050.0 450.00 52.00 152.00 352.00]';


% Temperature (K)


X(:,2)=[303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323 323 323
323 323 323 323 303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323
323 323 323 323 323 323 303 303 303 303 303 303 303 313 313 313 313 313 313 313 323
323 323 323 323 323 323 313 313 313 313 313 313 313 313 313 313 313 313 313 313 313
313 313 313 313 313 313 313 313 313 313 313 313 313 313 323 323 323 323 323 323
323 323 323 333 333 333 333 333 333 333 333 333 333 343 343 343 343 343 343 343 333
333 333 333 333 333 333 333 333 333 333 362.1 362.1 362.1 362.1 362.1 362.1 412.1 412.1
412.1 412.1 412.1 412.1 362.1 362.1 362.1 362.1 362.1 362.1 412.1 412.1 412.1 412.1 412.1
412.1]' ;
```

Appendix I

```
% Ratio of concentration (DEA:MDEA)

X(:,3)=[0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33
0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0
3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.33 0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00
1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.113 0.113 0.113 0.113 0.113 0.113 0.113
0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113
0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.068 0.068
0.068 0.068 0.068 0.227 0.227 0.227 0.227 0.227 0.227 1.143 1.143 1.143 1.143 1.143 1.143
1.143 1.143 1.143 1.143 1.143 1.143 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76
0.76]' ;

% y-value

y=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2 28.9
50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0 10.3
29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1 10.2
31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5 47.4
95.1 4.81 6.10 8.40 9.61 11.80 16.80 21.40 25.20 29.80 9.01 11.0 14.50 17.10 23.50 33.80
39.10 44.50 49.00 17.90 18.40 21.80 22.8 33.1 40.10 51.2 57.3 64.1 72.1 21.8 29.0 40.80
48.2 55.2 61.0 63.50 12.1 15.2 18.9 37.7 42.8 14.6 19.0 27.4 35.5 46.1 56.8 150.00 450.00
105.100 351.00 61.00 149.00 151.00 450.00 1153.00 49.00 160.00 351.00 450.0 1050.0
152.00 57.00 351.00 152.00 153.00 1050.0 450.00 52.00 152.00 352.00]' ;

% Normalization

[Z,MU,SIGMA] = zscore(X);

%Regression

LM = LinearModel.fit(Z,y,'linear') ;
```

Appendix II

```
% Mixture DEA and MDEA MLR

% by fareez 16/8/2013


%Data Input

X=zeros(158,3);


% CO2 Partial Pressure (kPa)

X(:,1)=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2
28.9 50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0
10.3 29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1
10.2 31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5
47.4 95.1 4.81 6.10 8.40 9.61 11.80 16.80 21.40 25.20 29.80 9.01 11.0 14.50 17.10 23.50
33.80 39.10 44.50 49.00 17.90 18.40 21.80 22.8 33.1 40.10 51.2 57.3 64.1 72.1 21.8 29.0
40.80 48.2 55.2 61.0 63.50 12.1 15.2 18.9 37.7 42.8 14.6 19.0 27.4 35.5 46.1 56.8 150.00
450.00 105.100 351.00 61.00 149.00 151.00 450.00 1153.00 49.00 160.00 351.00 450.0
1050.0 152.00 57.00 351.00 152.00 153.00 1050.0 450.00 52.00 152.00 352.00]';


% Temperature (K)

X(:,2)=[303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323 323 323
323 323 323 323 303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323
323 323 323 323 323 323 303 303 303 303 303 303 303 313 313 313 313 313 313 313 323
323 323 323 323 323 323 313 313 313 313 313 313 313 313 313 313 313 313 313 313 313
313 313 313 313 313 313 313 313 313 313 313 313 313 313 323 323 323 323 323 323
323 323 323 333 333 333 333 333 333 333 333 333 333 343 343 343 343 343 343 343 333
333 333 333 333 333 333 333 333 333 333 362.1 362.1 362.1 362.1 362.1 362.1 412.1 412.1
412.1 412.1 412.1 412.1 412.1 362.1 362.1 362.1 362.1 362.1 362.1 412.1 412.1 412.1 412.1 412.1
412.1]' ;


% Ratio of concentration (DEA:MDEA)

X(:,3)=[0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33
0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0
3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.33 0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00
1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.113 0.113 0.113 0.113 0.113 0.113 0.113
0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113
0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.068 0.068
0.068 0.068 0.068 0.227 0.227 0.227 0.227 0.227 0.227 1.143 1.143 1.143 1.143 1.143 1.143
```

Appendix II

1.143 1.143 1.143 1.143 1.143 1.143 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76]' ;

% y-value

y=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2 28.9 50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0 10.3 29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1 10.2 31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5 47.4 95.1 4.81 6.10 8.40 9.61 11.80 16.80 21.40 25.20 29.80 9.01 11.0 14.50 17.10 23.50 33.80 39.10 44.50 49.00 17.90 18.40 21.80 22.8 33.1 40.10 51.2 57.3 64.1 72.1 21.8 29.0 40.80 48.2 55.2 61.0 63.50 12.1 15.2 18.9 37.7 42.8 14.6 19.0 27.4 35.5 46.1 56.8 150.00 450.00 105.100 351.00 61.00 149.00 151.00 450.00 1153.00 49.00 160.00 351.00 450.0 1050.0 152.00 57.00 351.00 152.00 153.00 1050.0 450.00 52.00 152.00 352.00]' ;

% Normalization

[Z,MU,SIGMA] = zscore(X);

%Regression

LM = LinearModel.fit(Z,y,'quadratic') ;

Appendix III

```
% Mixture DEA and MDEA MLR

% by fareez 12/7/2013


%Data Input

X=zeros(88,3);


% CO2 Partial Pressure (kPa)

X(:,1)=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2
28.9 50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0
10.3 29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1
10.2 31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5
47.4 95.1]';


% Temperature (K)

XT=[303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323 323 323 323
323 323 323 303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323 323
323 323 323 323 323 303 303 303 303 303 303 303 313 313 313 313 313 313 313 323 323
323 323 323 323 313 313 313 313 313 313 313 313 313 313 313 313 313 313 313 313 313
313 313 313 313 313]' ;


X(:,2)= 1./XT ;


% Ratio of concentration (DEA:MDEA)

X(:,3)=[0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33
0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0
3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.33 0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00
1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0]' ;


% y-value

y=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2 28.9
50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0 10.3
29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1 10.2
```

Appendix III

```
31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5 47.4
95.1]' ;


% Normalization

[Z,MU,SIGMA] = zscore(X);


%Regression

LM = LinearModel.fit(Z,y,'quadratic') ;
```

Appendix IV

```
% Artificial Neural Network (ANN)

% Mixture DEA and MDEA MLR

% by fareez 19/8/2013


%Data Input

X=zeros(158,3);


% CO2 Partial Pressure (kPa)

X(:,1)=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2
28.9 50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0
10.3 29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1
10.2 31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5
47.4 95.1 4.81 6.10 8.40 9.61 11.80 16.80 21.40 25.20 29.80 9.01 11.0 14.50 17.10 23.50
33.80 39.10 44.50 49.00 17.90 18.40 21.80 22.8 33.1 40.10 51.2 57.3 64.1 72.1 21.8 29.0
40.80 48.2 55.2 61.0 63.50 12.1 15.2 18.9 37.7 42.8 14.6 19.0 27.4 35.5 46.1 56.8 150.00
450.00 105.100 351.00 61.00 149.00 151.00 450.00 1153.00 49.00 160.00 351.00 450.0
1050.0 152.00 57.00 351.00 152.00 153.00 1050.0 450.00 52.00 152.00 352.00]';


% Temperature (K)

X(:,2)=[303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323 323 323
323 323 323 323 303 303 303 303 303 303 303 303 313 313 313 313 313 313 313 313 323
323 323 323 323 323 323 303 303 303 303 303 303 303 313 313 313 313 313 313 313 323
323 323 323 323 323 323 313 313 313 313 313 313 313 313 313 313 313 313 313 313 313
313 313 313 313 313 313 313 313 313 313 313 313 313 313 323 323 323 323 323 323
323 323 323 333 333 333 333 333 333 333 333 333 333 343 343 343 343 343 343 343 333
333 333 333 333 333 333 333 333 333 333 362.1 362.1 362.1 362.1 362.1 362.1 412.1 412.1
412.1 412.1 412.1 412.1 362.1 362.1 362.1 362.1 362.1 362.1 412.1 412.1 412.1 412.1 412.1
412.1]' ;


% Ratio of concentration (DEA:MDEA)

X(:,3)=[0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33 0.33
0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0
3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.33 0.33 0.33 0.33 0.33 0.33 0.33 1.00 1.00 1.00
1.00 1.00 1.00 1.00 3.0 3.0 3.0 3.0 3.0 3.0 3.0 0.113 0.113 0.113 0.113 0.113 0.113 0.113
0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113
```

Appendix IV

0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.113 0.068 0.068 0.068 0.068 0.068 0.227 0.227 0.227 0.227 0.227 0.227 1.143 1.143 1.143 1.143 1.143 1.143 1.143 1.143 1.143 1.143 1.143 1.143 1.143 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76 0.76]' ;

% y-value

y=[.1 .6 1.1 5.4 10.8 33.2 55.1 107.1 .1 .5 1.1 5.3 10.6 32.1 53.2 102.8 .1 1.1 5.1 10.2 28.9 50.9 90.7 .1 .6 1.1 5.4 9.8 32.1 49.3 106.4 .1 .5 1.1 5.4 10.6 32.3 53.0 102.1 .1 1.0 5.0 10.3 29.3 50.8 97.7 .1 1.1 5.5 10.9 33.2 55.1 106.4 .1 1.1 5.4 10.7 31.9 53.9 103.8 .1 1.0 5.1 10.2 31.0 50.1 101.0 .1 .9 4.8 9.8 28.5 47.6 95.1 .1 .9 4.8 9.5 28.6 47.4 94.1 .1 .9 4.8 9.5 28.5 47.4 95.1 4.81 6.10 8.40 9.61 11.80 16.80 21.40 25.20 29.80 9.01 11.0 14.50 17.10 23.50 33.80 39.10 44.50 49.00 17.90 18.40 21.80 22.8 33.1 40.10 51.2 57.3 64.1 72.1 21.8 29.0 40.80 48.2 55.2 61.0 63.50 12.1 15.2 18.9 37.7 42.8 14.6 19.0 27.4 35.5 46.1 56.8 150.00 450.00 105.100 351.00 61.00 149.00 151.00 450.00 1153.00 49.00 160.00 351.00 450.0 1050.0 152.00 57.00 351.00 152.00 153.00 1050.0 450.00 52.00 152.00 352.00]' ;

% Normalization

[Z,MU,SIGMA] = zscore(X);

Appendix V

T(K)	P_{CO2} (kPa)	DEA (kmol/m3)	MDEA (kmol/m3)	α_{CO2} (exp)	α_{CO2}(calc)	Deviation
303	0.1	0.5	1.5	0.079	0.275817391	-0.197
303	0.6	0.5	1.5	0.153	0.279983885	-0.127
303	1.1	0.5	1.5	0.214	0.284147945	-0.070
303	5.4	0.5	1.5	0.426	0.319846768	0.106
303	10.8	0.5	1.5	0.535	0.364337538	0.171
303	33.2	0.5	1.5	0.706	0.542887852	0.163
303	55.1	0.5	1.5	0.766	0.704054151	0.062
303	107.1	0.5	1.5	0.853	1.014241508	-0.161
313	0.1	0.5	1.5	0.065	0.155695686	-0.091
313	0.5	0.5	1.5	0.119	0.158837355	-0.040
313	1.1	0.5	1.5	0.161	0.163551135	-0.003
313	5.3	0.5	1.5	0.348	0.196580517	0.151
313	10.6	0.5	1.5	0.449	0.238294102	0.211
313	32.1	0.5	1.5	0.613	0.406205454	0.207
313	53.2	0.5	1.5	0.702	0.56509204	0.137
313	102.8	0.5	1.5	0.764	0.892089525	-0.128
323	0.1	0.5	1.5	0.043	0.127654534	-0.085
323	1.1	0.5	1.5	0.121	0.134287934	-0.013
323	5.1	0.5	1.5	0.257	0.160895912	0.096
323	10.2	0.5	1.5	0.340	0.194961231	0.145
323	28.9	0.5	1.5	0.501	0.320364104	0.181
323	50.9	0.5	1.5	0.629	0.466222212	0.163
323	90.7	0.5	1.5	0.724	0.714384081	0.010
303	0.1	1.0	1.0	0.116	0.328526834	-0.213
303	0.6	1.0	1.0	0.210	0.332048555	-0.122
303	1.1	1.0	1.0	0.292	0.335562674	-0.044
303	5.4	1.0	1.0	0.477	0.365459538	0.112
303	9.8	1.0	1.0	0.538	0.395415819	0.143
303	32.1	1.0	1.0	0.698	0.535737852	0.162
303	49.3	1.0	1.0	0.730	0.628675643	0.101
303	106.4	1.0	1.0	0.802	0.82419321	-0.022
313	0.1	1.0	1.0	0.071	0.2564307	-0.185
313	0.5	1.0	1.0	0.165	0.25927235	-0.094
313	1.1	1.0	1.0	0.219	0.263530163	-0.045
313	5.4	1.0	1.0	0.370	0.293869482	0.076
313	10.6	1.0	1.0	0.485	0.330098665	0.155
313	32.3	1.0	1.0	0.604	0.474094155	0.130
313	53	1.0	1.0	0.677	0.596953514	0.080
313	102.1	1.0	1.0	0.764	0.810183626	-0.046
323	0.1	1.0	1.0	0.045	0.260657149	-0.216

Appendix V

T(K)	P_{CO2}, (kPa)	DEA (kmol/m3)	MDEA (kmol/m3)	α_{CO2} (exp)	α_{CO2}(calc)	Deviation
323	1	1.0	1.0	0.160	0.266247892	-0.106
323	5	1.0	1.0	0.304	0.290994145	0.013
323	10.3	1.0	1.0	0.378	0.323489122	0.055
323	29.3	1.0	1.0	0.514	0.436262001	0.078
323	50.8	1.0	1.0	0.603	0.554128384	0.049
323	97.7	1.0	1.0	0.670	0.759209994	-0.089
303	0.1	1.5	0.5	0.239	0.312190134	-0.073
303	1.1	1.5	0.5	0.328	0.318817985	0.009
303	5.5	1.5	0.5	0.493	0.347532288	0.145
303	10.9	1.5	0.5	0.575	0.381749204	0.193
303	33.2	1.5	0.5	0.691	0.510535728	0.180
303	55.1	1.5	0.5	0.764	0.61702643	0.147
303	106.4	1.5	0.5	0.810	0.795642269	0.014
313	0.1	1.5	0.5	0.145	0.243118115	-0.098
313	1.1	1.5	0.5	0.271	0.250044554	0.021
313	5.4	1.5	0.5	0.421	0.279500403	0.141
313	10.7	1.5	0.5	0.478	0.315046014	0.163
313	31.9	1.5	0.5	0.609	0.448106466	0.161
313	53.9	1.5	0.5	0.692	0.569569641	0.122
313	103.8	1.5	0.5	0.764	0.781422443	-0.017
323	0.1	1.5	0.5	0.071	0.258823484	-0.188
323	1	1.5	0.5	0.206	0.264363583	-0.058
323	5.1	1.5	0.5	0.353	0.289412055	0.064
323	10.2	1.5	0.5	0.422	0.320123519	0.102
323	31	1.5	0.5	0.553	0.439934311	0.113
323	50.1	1.5	0.5	0.606	0.541803186	0.064
323	101	1.5	0.5	0.682	0.772921285	-0.091
313	0.1	1.0	3.0	0.038	0.155695686	-0.118
313	0.9	1.0	3.0	0.121	0.161979711	-0.041
313	4.8	1.0	3.0	0.268	0.192646186	0.075
313	9.8	1.0	3.0	0.306	0.231998297	0.074
313	28.5	1.0	3.0	0.465	0.378374657	0.087
313	47.6	1.0	3.0	0.525	0.523762343	0.001
313	95.1	1.0	3.0	0.632	0.846703061	-0.215
313	0.1	2.0	2.0	0.063	0.2564307	-0.193
313	0.9	2.0	2.0	0.175	0.26211152	-0.087
313	4.8	2.0	2.0	0.322	0.289655489	0.032
313	9.5	2.0	2.0	0.385	0.322480571	0.063
313	28.6	2.0	2.0	0.503	0.450505295	0.052
313	47.4	2.0	2.0	0.540	0.565364206	-0.025

Appendix V

T(K)	P_{CO2}, (kPa)	DEA (kmol/m3)	MDEA (kmol/m3)	α_{CO2} (exp)	α_{CO2}(calc)	Deviation
313	94.1	2.0	2.0	0.609	0.78395155	-0.175
313	0.1	3.0	1.0	0.073	0.243118115	-0.170
313	0.9	3.0	1.0	0.181	0.248661527	-0.068
313	4.8	3.0	1.0	0.371	0.275422794	0.096
313	9.5	3.0	1.0	0.441	0.30707353	0.134
313	28.5	3.0	1.0	0.517	0.427795423	0.089
313	47.4	3.0	1.0	0.579	0.535497304	0.044
313	95.1	3.0	1.0	0.632	0.75057131	-0.119
313	4.81	0.305	2.695	0.107	0.174917161	-0.068
313	6.1	0.305	2.695	0.137	0.185396735	-0.048
313	8.4	0.305	2.695	0.165	0.204109098	-0.039
313	9.61	0.305	2.695	0.189	0.213965807	-0.025
313	11.8	0.305	2.695	0.236	0.231823279	0.004
313	16.8	0.305	2.695	0.275	0.272649993	0.002
313	21.4	0.305	2.695	0.319	0.31022975	0.009
313	25.2	0.305	2.695	0.356	0.341246945	0.015
313	29.8	0.305	2.695	0.391	0.378713987	0.012
323	9.01	0.305	2.695	0.135	0.138212547	-0.003
323	11	0.305	2.695	0.167	0.151928302	0.015
323	14.5	0.305	2.695	0.201	0.176147269	0.025
323	17.1	0.305	2.695	0.223	0.194208945	0.029
323	23.5	0.305	2.695	0.283	0.238876042	0.044
323	33.8	0.305	2.695	0.320	0.311162073	0.009
323	39.1	0.305	2.695	0.359	0.348431941	0.011
323	44.5	0.305	2.695	0.398	0.386380573	0.012
323	49	0.305	2.695	0.431	0.417944653	0.013
333	17.9	0.305	2.695	0.128	0.143066332	-0.015
333	18.4	0.305	2.695	0.160	0.146009126	0.014
333	21.8	0.305	2.695	0.192	0.166054633	0.026
333	22.8	0.305	2.695	0.218	0.171960534	0.046
333	33.1	0.305	2.695	0.271	0.232960364	0.038
333	40.1	0.305	2.695	0.301	0.274468586	0.027
333	51.2	0.305	2.695	0.334	0.340079631	-0.006
333	57.3	0.305	2.695	0.361	0.37590972	-0.015
333	64.1	0.305	2.695	0.390	0.415576762	-0.026
333	72.1	0.305	2.695	0.427	0.46178764	-0.035
343	21.8	0.305	2.695	0.127	0.096403831	0.031
343	29	0.305	2.695	0.194	0.134814385	0.059
343	40.8	0.305	2.695	0.235	0.197525635	0.037
343	48.2	0.305	2.695	0.261	0.236478997	0.025

Appendix V

T(K)	P_{CO2}, (kPa)	DEA (kmol/m3)	MDEA (kmol/m3)	α_{CO2} (exp)	α_{CO2}(calc)	Deviation
343	55.2	0.305	2.695	0.295	0.272919955	0.022
343	61	0.305	2.695	0.317	0.302743628	0.014
343	63.5	0.305	2.695	0.326	0.315481818	0.011
333	12.1	0.191	2.809	0.055	0.099792177	-0.045
333	15.2	0.191	2.809	0.099	0.118159002	-0.019
333	18.9	0.191	2.809	0.130	0.140178818	-0.010
333	37.7	0.191	2.809	0.241	0.25306675	-0.012
333	42.8	0.191	2.809	0.280	0.283788875	-0.004
333	14.6	0.555	2.445	0.111	0.151170744	-0.040
333	19	0.555	2.445	0.160	0.176339841	-0.016
333	27.4	0.555	2.445	0.231	0.224490467	0.007
333	35.5	0.555	2.445	0.280	0.270887322	0.009
333	46.1	0.555	2.445	0.331	0.3312704	0.000
333	56.8	0.555	2.445	0.370	0.391526943	-0.022
362.1	150	2.4	2.1	0.107	0.23432021	-0.127
362.1	450	2.4	2.1	0.296	0.361547271	-0.066
362.1	105.1	2.4	2.1	0.789	0.26921722	0.520
362.1	351	2.4	2.1	0.297	0.253404281	0.044
362.1	61	2.4	2.1	0.043	0.234313915	-0.191
362.1	149	2.4	2.1	0.101	0.235534998	-0.135
412.1	151	2.4	2.1	0.098	-0.022718267	0.121
412.1	450	2.4	2.1	0.304	0.306197893	-0.002
412.1	1153	2.4	2.1	0.544	0.257093727	0.287
412.1	49	2.4	2.1	0.042	0.086808361	-0.045
412.1	160	2.4	2.1	0.102	-0.033028171	0.135
412.1	351	2.4	2.1	0.200	0.104416938	0.096
362.1	450	1.9	2.5	0.293	0.250484821	0.043
362.1	1050	1.9	2.5	0.301	0.302613542	-0.002
362.1	152	1.9	2.5	0.117	0.203570041	-0.087
362.1	57	1.9	2.5	0.046	0.03899418	0.007
362.1	351	1.9	2.5	0.344	0.05116639	0.293
362.1	152	1.9	2.5	0.148	0.203570041	-0.056
412.1	153	1.9	2.5	0.094	0.127408778	-0.033
412.1	1050	1.9	2.5	0.301	0.301602257	-0.001
412.1	450	1.9	2.5	0.236	0.341941364	-0.106
412.1	52	1.9	2.5	0.043	0.051146505	-0.008
412.1	152	1.9	2.5	0.155	0.127709857	0.027
412.1	352	1.9	2.5	0.209	0.207833316	0.001

Appendix VI

T(K)	P_{CO2} (kPa)	DEA (kmol/m3)	MDEA (kmol/m3)	α_{CO2} (exp)	α_{CO2}(calc)	Deviation
303	1.1	2.0	0.0	0.388	0.321447988	0.067
303	5.4	2.0	0.0	0.521	0.476092848	0.045
303	10.7	2.0	0.0	0.593	0.592439864	0.001
303	32.5	2.0	0.0	0.699	0.684016703	0.015
303	54.2	2.0	0.0	0.73	0.706935315	0.023
303	100.9	2.0	0.0	0.786	0.761923389	0.024
313	0.1	2.0	0.0	0.172	0.223985468	-0.052
313	0.5	2.0	0.0	0.278	0.241898831	0.036
313	1	2.0	0.0	0.32	0.263560183	0.056
313	5.3	2.0	0.0	0.459	0.416054054	0.043
313	10.7	2.0	0.0	0.538	0.531620468	0.006
313	32.1	2.0	0.0	0.597	0.610598882	-0.014
313	53.8	2.0	0.0	0.662	0.661795180	0.000
313	104.7	2.0	0.0	0.727	0.738526990	-0.012
323	0.1	2.0	0.0	0.133	0.145289859	-0.012
323	0.5	2.0	0.0	0.152	0.164120252	-0.012
323	1	2.0	0.0	0.272	0.186910846	0.085
323	5.1	2.0	0.0	0.398	0.342223840	0.056
323	10	2.0	0.0	0.473	0.461338586	0.012
323	30.4	2.0	0.0	0.546	0.567405857	-0.021
323	50.8	2.0	0.0	0.611	0.601230048	0.010
323	98.2	2.0	0.0	0.688	0.691887149	-0.004
303	0.1	4.0	0.0	0.122	0.190675765	-0.069
303	1	4.0	0.0	0.309	0.229332315	0.080
303	4.9	4.0	0.0	0.471	0.376322206	0.095
303	9.9	4.0	0.0	0.524	0.506277237	0.018
303	29.4	4.0	0.0	0.588	0.644853063	-0.057
303	48.9	4.0	0.0	0.633	0.640786806	-0.008
303	98.6	4.0	0.0	0.671	0.759108360	-0.088
313	0.1	4.0	0.0	0.091	0.168039894	-0.077
313	0.9	4.0	0.0	0.281	0.199785193	0.081
313	5.3	4.0	0.0	0.441	0.343563821	0.097
313	10.4	4.0	0.0	0.499	0.450809920	0.048
313	31	4.0	0.0	0.561	0.588854740	-0.028
313	52.6	4.0	0.0	0.599	0.549833834	0.049
313	102.1	4.0	0.0	0.639	0.649447464	-0.010
323	0.1	4.0	0.0	0.091	0.137275630	-0.046
323	0.9	4.0	0.0	0.193	0.161826759	0.031
323	4.5	4.0	0.0	0.344	0.251652388	0.092

Appendix VII

T(K)	P_{CO2} (kPa)	DEA (kmol/m3)	MDEA (kmol/m3)	α_{CO2} (exp)	α_{CO2}(calc)	Deviation
303	4.8	0.0	2.0	0.333	0.182	0.151
303	10.5	0.0	2.0	0.483	0.307	0.176
303	29.8	0.0	2.0	0.673	0.635	0.038
303	48.4	0.0	2.0	0.793	0.736	0.057
303	95.8	0.0	2.0	0.88	0.766	0.114
313	1.1	0.0	2.0	0.103	0.110	-0.007
313	3.1	0.0	2.0	0.197	0.168	0.029
313	5.2	0.0	2.0	0.267	0.228	0.039
313	10	0.0	2.0	0.974	0.355	0.619
313	30.3	0.0	2.0	0.603	0.667	-0.064
313	47.5	0.0	2.0	0.688	0.736	-0.048
313	94	0.0	2.0	0.805	0.753	0.052
323	1	0.0	2.0	0.079	-0.045	0.124
323	2.9	0.0	2.0	0.148	0.003	0.145
323	4.8	0.0	2.0	0.194	0.049	0.145
323	9.7	0.0	2.0	0.298	0.159	0.139
323	28.4	0.0	2.0	0.471	0.470	0.001
323	44.1	0.0	2.0	0.59	0.629	-0.039
323	91.5	0.0	2.0	0.726	0.725	0.001
303	0.1	0.0	4.0	0.027	0.130	-0.103
303	1	0.0	4.0	0.061	0.149	-0.088
303	4.9	0.0	4.0	0.149	0.233	-0.084
303	9.8	0.0	4.0	0.284	0.329	-0.045
303	29.5	0.0	4.0	0.516	0.553	-0.037
303	49.1	0.0	4.0	0.633	0.630	0.003
303	98.2	0.0	4.0	0.761	0.739	0.022
313	0.1	0.0	4.0	0.015	0.011	0.004
313	0.9	0.0	4.0	0.052	0.032	0.020
313	4.8	0.0	4.0	0.085	0.129	-0.044
313	9.5	0.0	4.0	0.190	0.233	-0.043
313	28.5	0.0	4.0	0.384	0.484	-0.100
313	47.5	0.0	4.0	0.513	0.560	-0.047
313	95.2	0.0	4.0	0.654	0.666	-0.012
323	0.1	0.0	4.0	0.01	-0.001	0.011
323	0.9	0.0	4.0	0.037	0.011	0.026
323	4.5	0.0	4.0	0.084	0.059	0.025
323	9	0.0	4.0	0.151	0.107	0.044
323	27.1	0.0	4.0	0.251	0.226	0.025
323	45.1	0.0	4.0	0.363	0.356	0.007